Георгий Михайлович Жидомиров

(11.07.1933– 31.07.2019)

Ушел из жизни Георгий Михайлович Жидомиров - специалист в области прикладной квантовой химии, теоретической спектроскопии и теории гетерогенного и металлокомплексного катализа. Доктор физико-математических наук (1977), профессор (1986), Заслуженный деятель науки РФ (1999), академик Российской академии естественных наук, Зав. лабораторией квантовой химии (1982-2003), с 2003 г. главный научный сотрудник, Заслуженный профессор Института катализа.

Георгий Михайлович Жидомиров родился в 1933г. в г. Иваново. Начал свой научный путь в коллективе академика В.В. Воеводского, куда был приглашен после окончания МИФИ в 1958 г. для работы в области теории ЭПР свободных радикалов. Первые исследования Г.М. Жидомирова были посвящены теории спин-решеточной релаксации свободных радикалов в молекулярных кристаллах, где он нашел эффективный релаксационный механизм, связанный с взаимодействием с ориентационными фононами.

В 1960 г. Г.М. Жидомиров переехал на работу в Новосибирский Академгородок в Институт химической кинетики и горения СО АН СССР. Здесь он начал вместе с П.В. Счастневым первые в отечественной науке систематические квантово-химические расчеты магнитно-резонансных параметров (МРП) свободных радикалов. Для проведения этих исследований Г.М. Жидомировым и его сотрудниками была проведена большая работа по модификации и развитию расчетных методов и разработке соответствующего программного обеспечения. Были проведены расчеты распределения спиновой плотности и констант сверхтонкого взаимодействия (СТВ) в свободных радикалах различных структурных классов, проанализирована сравнительная роль спиновой делокализации и спиновой поляризации.

В 1964 г. Георгий Михайлович защитил кандидатскую диссертацию «Спектры ЭПР и спин-решеточная релаксация радикалов в некоторых твердых матрицах».

Другим направлением научных интересов Г.М. Жидомирова в этот период была теория электронного спинового эха свободных радикалов в замороженных растворах. Экспериментальные исследования в этой области стали возможны после создания в ИХКиГ А.Г. Семеновым и В.Е. Хмелинским ЭПР-релаксометра и были начаты в середине 60-х в лаборатории Ю.Д. Цветкова. В задачу Г.М. Жидомирова и вскоре присоединившегося к нему К.М. Салихова входила теоретическая интерпретация экспериментальных результатов в этой только формирующейся области исследований. Ими были проведены первые теоретические исследования, посвященные как расчетам параметров спада спинового эха свбодных радикалов, так и осцилляционной модуляции кривых спада.

В 1967 г. после преждевременной кончины академика В.В. Воеводского Г.М. Жидомиров переезжает по предложению профессора В.Б. Казанского на работу в Москву в Институт органической химии АН СССР. В этот период им продолжаются исследования в области теории МРП свободных радикалов, в частности, начаты одни из первых в литературе расчеты *g*-тензоров, делокализации спиновой плотности на молекулы сольватов в растворах и предложена интерпретация корреляционных соотношений между МРП в молекулах, радикалах и парамагнитных комплексах с органическими лигандами. Итоги всех этих многолетних исследований были подведены в монографии «Квантово-химические расчеты магнитно-резонансных параметров. Свободные радикалы», Новосибирск, Наука, 1978 г. (совместно с П.В. Счастневым и Н.Д. Чувылкиным).

Другим важным направлением работ Г.М. Жидомирова в области теории радиоспектроскопии была разработка методов расчетного синтеза спектров ЭПР, форма которых определяется наложением тонкого, сверхтонкого и спин-орбитального взаимодействий. К этому же разделу примыкают исследования изменения формы спектров ЭПР, обусловленные анизотропными (в том числе квантовыми) усредняющими движениями парамагнитной частицы в матрице и формы спектров бирадикалов в условиях динамического спинового обмена. Эти исследования нашли отражение в монографиях «Интерпретация сложных спектров ЭПР», Москва, Наука, 1975 г. (совместно с Я.С. Лебедевым, С.Н. Добряковым, Н.Я. Штейшнейдером, А.К. Чирковым и В.А. Губановым) и «Стабильные бирадикалы», Москва, Наука, 1980 г. (совместно с В.Н. Пармоном и А.И. Кокориным). По результатам этих исследований им была защищена докторская диссертация «Квантово-механические расчеты магнитно-резонансных параметров».

С середины 70-х главной темой исследований Г.М. Жидомирова стала теория гетерогенного катализа. Им было начато широкое применение кластерного подхода в расчетах структуры и спектральных характеристик хемосорбционных комплексов и элементарных актов каталитических процессов на поверхности твердых катализаторов. Первый этап этой работы состоял в систематическом исследовании Бренстедовских и Льюисовских кислотных центров цеолитов и аморфных алюмосиликатов. Эти исследования были им продолжены и после перехода по предложению академика Г.К. Борескова на работу в Институт катализа СО АН СССР в 1982 г., где Г.М. Жидомиров организовал лабораторию квантовой химии. Были проанализированы химические и структурные факторы, влияющие на каталитическую активность центров и показана важная роль нежесткости поверхности катализатора при рассмотрении хемосорбции и каталитических реакций, а также определяющая важность кулоновских взаимодействий в реализующейся ионной паре при образовании интермедиатов и переходных состояний кислотного катализа в цеолитах. Кластерный подход был успешно применен в задачах о формировании цеолитов и их модификации при термо-вакуумной и термохимической обработках, что позволило проследить механизм образования активных кислотных центров в цеолитах и предложить пути модификации их каталитических свойств. Итоги этих исследований были частично подведены в монографии «Кластерное приближение в квантовохимических исследованиях хемосорбции и поверхностных структур. Строение молекул и химическая связь». (Итоги науки и техники, ВИНИТИ АН СССР), 1984 г., т.9 (совместно с И.Д. Михейкиным) и в обзорах G.M. Zhidomirov, V.B. Kazansky “Quantum chemical

cluster Models of acid-base sites of oxide catalysts". Adv. In Catal., 34 (1986) 131-202 и К.И. Замараев, Г.М. Жидомиров. «Активные центры и роль среды в гомогенном, гетерогенном и ферментативном катализе: сходство и различие». Труды Международного симпозиума по связи между гомогенным и гетерогенным катализом. Сб. докладов т.1 (1986), 24-68, Новосибирск.

Для методического обеспечения исследований в лаборатории квантовой химии ИК СО РАН в эти годы были разработаны полуэмпирические программы квантово-химического расчета химических свойств поверхности оксидов непереходных (MINDO/3-HB) и переходных элементов (NDDO/MC); расчета магнитно-резонансных параметров спектров ЭПР (Spin-Hamiltonian), электронных спектров (X_α - Omega) и спектров XAFS (X_α - continuous), расчета формы анизотропно-уширенных спектров ЭПР (ESR1, ESR2, BIRAD); статических и MAS спектров ЯМР квадрупольных ядер (SATRAS).

В последующем цеолиты оставались одним из главных приоритетов в работах Г.М. Жидомирова, однако предметом исследований являлись уже хемосорбционные и каталитические свойства катионов металлов, стабилизированных в цеолитной матрице. В расчетном плане важной компонентой успеха этих работ оказался удачный подход к заданию граничных условий в кластерных моделях выделенных структур в цеолитах, который позволил проводить квантовохимические расчеты взаимодействия реагентов активных центров с оптимизацией геометрии адсорбционного комплекса (учетом релаксации решетки) при оптимальном соответствии начальной геометрии кластера известным экспериментальным параметрам структуры катализатора. Развитые подходы показали свою эффективность в расчетах сравнительной стабильности различных структурных форм катионов металлов в цеолитах и были применены при квантовохимических исследованиях активности Zn/HZSM-5 и Ga/HZSM-5 (реакция дегидрирования алканов) и FeZSM-5 (прямое окисление бензола в фенол закисью азота) цеолитов, а также при моделировании активных центров V_2O_5/TiO_2 нанесенных катализаторов. В молекулярном моделировании каталитических центров в катион-содержащих цеолитах особую проблему составлял случай стабилизации многовалентных катионов в высококремнистых цеолитах. Были систематически рассмотрены особенности стабилизации 2-х- и 3-х- валентных катионов металлов. В работах Г.М. Жидомирова и его сотрудников были впервые построены реалистические кластерные модели биядерных мостиковых структур $(Zn\text{-}O\text{-}Zn)^{2+}$, $(Fe\text{-}O\text{-}Fe)^{2+}$ в ZSM-5 для этого случая и рассмотрена их реакционная способность. Впервые теоретически предсказана возможность формирования суперактивных центров в ZnZSM-5, которые позволили объяснить как экспериментально наблюдаемые аномально большие сдвиги колебательных полос H_2 и CH_4 при их молекулярной хемосорбции в Zn-содержащих MFI цеолитах, так и последующую их диссоциацию при повышении температуры. Были рассмотрены пути формирования и стабилизации в Zn/HZSM-5 и Ga/HZSM-5 оксидных нано-кластеров Zn и Ga и показано, что предварительное частичное гидрирование кластеров необходимо для их активности в каталитическом процессе дегидрирования легких алканов. Расчетным путем было найдено, что биядерные мостиковые структуры катионов щелочноземельных металлов в морденитах и фажазитах могут накапливать кислород с формированием структур типа $[CaO_nCa]^{2+}$, n=2-4, что позволило объяснить экспериментально наблюдаемое накопление кислорода в цеолитах и выделение синглетного кислорода при нагревании. Высказано предположение, что через такие структуры могут идти процессы окисления молекулярным кислородом.
Результаты этихи следований частично представлены в обзорах G.M. Zhidomirov, A.A. Shubin, R.A. vanSanten "Structure and Reactivity of MetalIon Species in High Silica Zeolites". Chapter 7 in book: "Computer Modelling of Microporous Materials", Eds. C.R.A. Catlow, R.A. van Santen, B. Smit, Elsevier, Academii Pu11, London, p. 201-241 (2004) и G.M. Zhidomirov, A.A. Shubin, A.N. Larin, S.E. Malykhin, A.A. Rybakov "Molecular Models of the Stabilization of Bivalent Metal Cations in Zeolite Catalysts. In Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends". Ed. Prof. Jerzy Leszczynski, Dr. Manoj K. Shukla, Prof. Helene de Rode, Springer, (2011), in press.

Тематика исследований Г.М. Жидомирова и возглавлявшегося им коллектива сотрудников

охватывала широкий круг проблем теории катализа. Это и известная проблема сильного взаимодействия металла с носителем в нанесенных системах, когда были построены первые модели электронно-дефицитных частиц Pt и Pd в цеолитах, и обсуждение роли дефектов в хемосорбции и катализе на примере низко-координированных ионов поверхности оксидов магния и цинка. Отдельное направление составило моделирование вакансионных дефектов на поверхности серебра, для которых была предсказана стабилизация квазимолекулярных кислородных структур, активных в эпоксидировании этилена.

Г.М. Жидомиров автор и соавтор 465 статей в научных журналах, 25 обзоров и 5 монографий. Среди его учеников 27 кандидатов наук и 5 защитили докторские диссертации.

Г.М. Жидомиров являлся членом Совета директоров Международного общества по теоретической химической физике, он был заместителем главного редактора «Журнала структурной химии», членом редакции журнала «Кинетика и катализ».

По материалам http://catalysis.ru/block/index.php?ID=1&SECTION_ID=1449

Научные публикации Г.М. Жидомирова:

Монографии

1. Г.М. Жидомиров, Я.С. Лебедев, С.Н. Добряков, Н.Я. Штейншнейдер, А.К. Чирков, В.А. Губанов, Интерпретация сложных спектров ЭПР. Москва, Наука, 1975 [G.M.Zhidomirov, Ya.S.Lebedev, S.N.Dobryakov, N.Ya.Shteinshneider, A.K.Chirkov, V.A.Gubanov, Interpretation of complex ESR spectra, Oxonian Press PVT.LTD, New Delhi, Calcutta, 1985]
2. Г.М. Жидомиров, И.Д. Михейкин, Кластерное приближение в квантовохимических исследованиях хемосорбции и поверхностных структур. Строение молекул и химическая связь. Итоги науки и техники, ВИНИТИ АН СССР, 1984
3. В.Н. Пармон, А.И. Кокорин, Г.М. Жидомиров, Стабильные бирадикалы. Москва, Наука, 1980
4. Г.М. Жидомиров, А.А. Багатурьянц, И.А. Абронин, Прикладная квантовая химия. Расчеты реакционной способности и механизмов химических реакций. Москва, Химия, 1979
5. Г.М. Жидомиров, П.В. Счастнев, Н.Д. Чувылкин, Квантовохимические расчеты магнитно-резонансных параметров. Свободные радикалы. Новосибирск, Наука, 1978

Избранные статьи (по данным WebOfScience)

1. PAVLOVA, TV; SKOROKHODOV, ES; ZHIDOMIROV, GM; ELTSOV, KN.
   AB INITIO STUDY OF THE EARLY STAGE OF SI EPITAXY ON THE CHLORINATED SI(100) SURFACE
   JOURNAL OF PHYSICAL CHEMISTRY C 123(32), 19806-19811 (2019) AGARKOVA, EA;
2. GROMOV, OI; FEKLICHEV, ED; ZHIDOMIROV, GM; RYBALTOVSKII, AO; SVIRIDOV, AP; GRIGORIEV, YV; ISCHENKO, AA; BAGRATASHVILI, VN; GOLUBEVA, EN.
   INFLUENCE OF SOLVENT ELECTRON AFFINITY ON PARAMAGNETIC DEFECTS IN HYBRID SI/SIOX LUMINESCENT NANOPARTICLES
   JOURNAL OF NANOPARTICLE RESEARCH 21(6), - (2019)
3. RYBAKOV, AA; BRYUKHANOV, IA; LARIN, AV; TODOROVA, S; ZHIDOMIROV, GM.
   DIFFERENT LIMITS FOR CONVERGENT PD-PD LENGTHS IN PD SLABS GROWN OVER DIFFERENT OXIDES
   STRUCTURAL CHEMISTRY 30(2), 489-500 (2019)
4. ANDRYUSHECHKIN, BV; SHEVLYUGA, VM; PAVLOVA, TV; ZHIDOMIROV, GM; ELTSOV, KN.
   STM AND DFT STUDY OF CHLORINE ADSORPTION ON THE AG(111)-P(4 X 4)-O SURFACE
   JOURNAL OF PHYSICAL CHEMISTRY C 122(50), 28862-28867 (2018)
5. ZAVELEV, DE; ZHIDOMIROV, GM; TSODIKOV, MV.
   THEORETICAL STUDY OF INTERACTION BETWEEN HYDROGEN AND SMALL PT-SN INTERMETALLIC CLUSTERS
   KINETICS AND CATALYSIS 59(4), 405-417 (2018)
6. ANDRYUSHECHKIN, BV; SHEVLYUGA, VM; PAVLOVA, TV; ZHIDOMIROV, GM; ELTSOV, KN.

ADSORPTION OF MOLECULAR OXYGEN ON THE AG(111) SURFACE: A COMBINED TEMPERATURE-PROGRAMMED DESORPTION AND SCANNING TUNNELING MICROSCOPY STUDY
JOURNAL OF CHEMICAL PHYSICS 148(24), - (2018)

7. RYBAKOV, AA; BRYUKHANOV, IA; LARIN, AV; ZHIDOMIROV, GM.
THEORETICAL ANALYSIS OF OXIDATIVE CARBONYLATION OF METHANOL: SAEGUSA'S SCHEME OF DIMETHYLCARBONATE SYNTHESIS OVER BINUCLEAR CATIONIC OXO-CLUSTERS IN CUNAX ZEOLITE
JOURNAL OF PHYSICAL CHEMISTRY C 122(10), 5366-5375 (2018)
8. PAVLOVA, TV; ZHIDOMIROV, GM; ELTSOV, KN.
FIRST-PRINCIPLE STUDY OF PHOSPHINE ADSORPTION ON SI(001)-2 X 1-CL
JOURNAL OF PHYSICAL CHEMISTRY C 122(3), 1741-1745 (2018)
9. YULDASHEVA, G.; ZHIDOMIROV, G.; LESZCZYN-SKI, J.; ILIN, A..
IODINE CONTAINING DRUGS: COMPLEXES OF MOLECULAR IODINE AND TRI-IODIDE WITH BIO-ORGANIC LIGANDS AND LITHIUM HALOGENIDES IN AQUEOUS SOLUTIONS
PRACT ASP COMPUT CHEM. IV, 637 (2018)
10. STAROKON, EV; MALYKHIN, SE; PARFENOV, MV; ZHIDOMIROV, GM; KHARITONOV, AS.
OXIDATION OF LOWER ALKENES BY ALPHA-OXYGEN (FE-III-O CENTER DOT-)(ALPHA) ON THE FEZSM-5 SURFACE: THE EPOXIDATION OR THE ALLYLIC OXIDATION?
MOLECULAR CATALYSIS 443, 43-51 (2017)
11. MALKIN, VG; MALKINA, OL; ZHIDOMIROV, GM.
VISUALIZATION OF ELECTRON PARAMAGNETIC RESONANCE HYPERFINE STRUCTURE COUPLING PATHWAYS
JOURNAL OF PHYSICAL CHEMISTRY A 121(18), 3580-3587 (2017)
12. ANDRYUSHECHKIN, BV; SHEVLYUGA, VM; PAVLOVA, TV; ZHIDOMIROV, GM; ELTSOV, KN.
STRUCTURAL TRANSFORMATIONS ON AN OXIDIZED AG(111) SURFACE
JETP LETTERS 105(5), 292-296 (2017)
13. ANDRYUSHECHKIN, BV; SHEVLYUGA, VM; PAVLOVA, TV; ZHIDOMIROV, GM; ELTSOV, KN.
ADSORPTION OF O-2 ON AG(111): EVIDENCE OF LOCAL OXIDE FORMATION
PHYSICAL REVIEW LETTERS 117(5), - (2016)
14. RYBAKOV, AA; LARIN, AV; VERCAUTEREN, DP; ZHIDOMIROV, GM.
DFT MODELING OF PLASMA-ASSISTED ATOMIC LAYER DEPOSITION FOR SI(110) PASSIVATION: FORMATION OF BOEHMITE-LIKE CHAINS AS GAMMA-AL2O3 PRECURSORS
THEORETICAL CHEMISTRY ACCOUNTS 135(6), - (2016)
15. RYBAKOV, AA; BRYUKHANOV, IA; LARIN, AV; ZHIDOMIROV, GM.
THEORETICAL ASPECTS OF METHANOL CARBONYLATION ON COPPER-CONTAINING ZEOLITES
PETROLEUM CHEMISTRY 56(3), 259-266 (2016)
16. GOLUBEVA, EN; GROMOV, OI; ZHIDOMIROV, GM; ZUBANOVA, EM.
QUANTUM CHEMISTRY OF ORGANOCUPRATES AS INTERMEDIATES OF CATALYTIC AND PHOTOCHEMICAL REACTIONS
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 116(4), 295-300 (2016)
17. PAVLOVA, TV; ANDRYUSHECHKIN, BV; ZHIDOMIROV, GM.
FIRST-PRINCIPLE STUDY OF ADSORPTION AND DESORPTION OF CHLORINE ON CU(111) SURFACE: DOES CHLORINE OR COPPER CHLORIDE DESORB?
JOURNAL OF PHYSICAL CHEMISTRY C 120(5), 2829-2836 (2016)
18. CHERKEZ, VV; ZHELTOV, VV; DIDIOT, C; KIERREN, B; FAGOT-REVURAT, Y; MALTERRE, D; ANDRYUSHECHKIN, BV; ZHIDOMIROV, GM; ELTSOV, KN.
SELF-ORDERED NANOPOROUS LATTICE FORMED BY CHLORINE ATOMS ON AU(111)
PHYSICAL REVIEW B 93(4), - (2016)
19. ZAVELEV, DE; CHISTYAKOV, AV; ZHIDOMIROV, GM; GUBANOV, MA; TSODIKOV, MV; MOISEEV, II.
MECHANISM OF THE REDUCTIVE DEHYDRATION OF ETHANOL INTO C3+ ALKANES OVER THE COMMERCIAL ALUMINA-PLATINUM CATALYST AP-64
KINETICS AND CATALYSIS 57(1), 95-103 (2016)
20. RYBAKOV, AA; LARIN, AV; VERCAUTEREN, DP; ZHIDOMIROV, GM; LESZCZYNSKI, J; SHUKLA, MK.
PASSIVATION BY ATOMIC LAYER DEPOSITION OF AL2O3
PUBLISHER: SPRINGER US, BOSTON, MA , 303 (2016)
21. RYBAKOV, AA; BRYUKHANOV, IA; LARIN, AV; ZHIDOMIROV, GM.
CARBONATES IN ZEOLITES: FORMATION, PROPERTIES, REACTIVITY
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 115(24), 1709-1717 (2015)
22. ANDRYUSHECHKIN, BV; ZHELTOV, VV; CHERKEZ, VV; ZHIDOMIROV, GM; KLIMOV, AN; KIERREN, B; FAGOT-

REVURAT, Y; MALTERRE, D; ELTSOV, KN.
CHLORINE ADSORPTION ON CU(111) REVISITED: LT-STM AND DFT STUDY
SURFACE SCIENCE 639, 7-12 (2015)

23. MALYKHIN, SE; ANUFRIENKO, VF; HENSEN, EJM; KUZNETSOVA, EV; LARINA, TV; ZHIDOMIROV, GM.
DISTORTION OF THE TETRAHEDRAL COORDINATION OF FE(III) IONS STABILIZED IN ZSM-5 ZEOLITE FRAMEWORK (VOL 48, PG 855, 2007)
JOURNAL OF STRUCTURAL CHEMISTRY 56(4), 811-811 (2015)
24. KUZ'MIN, IV; SOKOLOVA, NA; SUBBOTINA, IR; ZHIDOMIROV, GM.
ETHYLENE ADSORPTION AND TRANSFORMATION ON ZEOLITE GA+/ZSM-5
RUSSIAN CHEMICAL BULLETIN 64(2), 278-283 (2015)
25. BRYUKHANOV, IA; RYBAKOV, AA; KOVALEV, VL; LARIN, AV; ZHIDOMIROV, GM.
CHEMICAL REDUCTION OF THE ELASTIC PROPERTIES OF ZEOLITES: A COMPARISON OF THE FORMATION OF CARBONATE SPECIES VERSUS DEALUMINATION
DALTON TRANSACTIONS 44(6), 2703-2711 (2015)
26. LARIN, AV; ZHIDOMIROV, GM.
STRUCTURE OF BI- AND TRINUCLEAR CLUSTERS OF ALUMINUM IONS AT THE CATIONIC SITES OF MORDENITE
JOURNAL OF STRUCTURAL CHEMISTRY 55(4), 583-594 (2014)
27. ZHELTOV, VV; CHERKEZ, VV; ANDRYUSHECHKIN, BV; ZHIDOMIROV, GM; KIERREN, B; FAGOT-REVURAT, Y; MALTERRE, D; ELTSOV, KN.
STRUCTURAL PARADOX IN SUBMONOLAYER CHLORINE COVERAGE ON AU(111)
PHYSICAL REVIEW B 89(19), - (2014)
28. RYBAKOV, AA; LARIN, AV; ZHIDOMIROV, GM.
INFLUENCE OF ALKALI CATIONS ON THE INTER-CONVERSION OF EXTRA-FRAMEWORK ALUMINIUM SPECIES IN DEALUMINATED ZEOLITES
MICROPOROUS AND MESOPOROUS MATERIALS 189, 173-180 (2014)
29. ZUBANOVA, EM; GOLUBEVA, EN; ZHIDOMIROV, GM.
TWO MECHANISMS OF CHLOROCUPRATE REACTIONS WITH ALKYL RADICALS: DRAMATIC ROLE OF NUCLEARITY
ORGANOMETALLICS 33(1), 121-128 (2014)
30. YULDASHEVA, GA; ZHIDOMIROV, GM; ILIN, AL.
THE ANTITUMOR ACTIVITY OF MOLECULAR IODINE COMPLEXES WITH LITHIUM HALOGENIDES AND BIOORGANIC LIGANDS WHEN APPLIED IN COMBINATION WITH DOXORUBICIN
J ANTIVIR ANTIRETROVIR 6, 50 (2014)
31. ANDRYUSHECHKIN, BV; CHERKEZ, VV; GLADCHENKO, EV; PAVLOVA, TV; ZHIDOMIROV, GM; KIERREN, B; DIDIOT, C; FAGOT-REVURAT, Y; MALTERRE, D; ELTSOV, KN.
SELF-ORGANIZATION OF GOLD CHLORIDE MOLECULES ON AU(111) SURFACE
JOURNAL OF PHYSICAL CHEMISTRY C 117(47), 24948-24954 (2013)
32. SUBBOTIN, AN; ZHIDOMIROV, GM; SUBBOTINA, IR; KAZANSKY, VB.
MOLECULAR AND DISSOCIATIVE ADSORPTION OF H2O ON ZEOLITE ZN/ZSM-5 STUDIED BY DIFFUSE-REFLECTANCE IR SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS
KINETICS AND CATALYSIS 54(6), 744-748 (2013)
33. SHILINA, MI; GLORIOZOV, IP; ZHIDOMIROV, GM.
QUANTUM CHEMICAL STUDY OF BUTANE METATHESIS ON MIXED ALUMINUM AND COBALT CHLORIDE COMPLEXES
RUSSIAN CHEMICAL BULLETIN 62(10), 2093-2101 (2013)
34. GOLUBEVA, EN; ZUBANOVA, EM; ZHIDOMIROV, GM.
THE NATURE OF CU-C BOND AND COPPER OXIDATION STATE IN CHLOROORGANOCUPRATES [CUCLNCH3]2-N
JOURNAL OF PHYSICAL ORGANIC CHEMISTRY 26(9), 724-729 (2013)
35. GROMOV, OI; GOLUBEVA, EN; ZHIDOMIROV, GM; MEL'NIKOV, MY.
COMPOUNDS WITH THE COPPER(II)-CARBON BOND: EPR SPECTROSCOPY AND QUANTUM CHEMISTRY
DOKLADY PHYSICAL CHEMISTRY 451, 154-156 (2013)
36. ZAVELEV, DE; ZHIDOMIROV, GM; KOZLOVSKII, RA.
QUANTUM CHEMICAL STUDY OF THE MECHANISM OF THE CATALYTIC OXYETHYLATION OF ETHYLENE GLYCOL ON PHOSPHORUS-DOPED TITANIUM DIOXIDE: THE ROLE OF THE SURFACE PHOSPHORYL AND HYDROXYL GROUPS OF THE CATALYST
KINETICS AND CATALYSIS 54(2), 157-167 (2013)
37. ANDRYUSHECHKIN, BV; CHERKEZ, VV; GLADCHENKO, EV; ZHIDOMIROV, GM; KIERREN, B; FAGOT-REVURAT, Y; MALTERRE, D; ELTSOV, KN.

NEW INSIGHT INTO THE STRUCTURE OF SATURATED CHLORINE LAYER ON AG(111): LT-STM AND DFT STUDY
APPLIED SURFACE SCIENCE 267, 21-25 (2013)

38. YULDASHEVA, GA; ZHIDOMIROV, GM; LESZCZYNSKI, J; ILIN, AI.
THE EFFECT OF THE AMPHOTERIC PROPERTIES OF AMINO ACIDS IN THE ZWITTERIONIC FORM ON THE STRUCTURE OF IODINE COMPLEX COMPOUNDS IN AQUEOUS SOLUTIONS
JOURNAL OF MOLECULAR STRUCTURE 1033, 321-330 (2013)
39. ANDRYUSHECHKIN, BV; CHERKEZ, VV; PAVLOVA, TV; ZHIDOMIROV, GM; ELTSOV, KN.
STRUCTURAL TRANSFORMATIONS OF CU(110) SURFACE INDUCED BY ADSORPTION OF MOLECULAR CHLORINE
SURFACE SCIENCE 608, 135-145 (2013)
40. GROMOV, OI; ZUBANOVA, EM; GOLUBEVA, EN; PLYUSNIN, VF; ZHIDOMIROV, GM; MELNIKOV, MY.
UV-VIS IDENTIFICATION AND DFT-ASSISTED PREDICTION OF STRUCTURES OF CU(II)-ALKYL CHLOROCOMPLEXES
JOURNAL OF PHYSICAL CHEMISTRY A 116(47), 11581-11585 (2012)
41. RYBAKOV, AA; LARIN, AV; ZHIDOMIROV, GM.
COMPUTATIONAL DIFFERENTIATION OF BRONSTED ACIDITY INDUCED BY ALKALINE EARTH OR RARE EARTH CATIONS IN ZEOLITES
INORGANIC CHEMISTRY 51(22), 12165-12175 (2012)
42. SHILINA, MI; GLORIOZOV, IP; ZHIDOMIROV, GM.
QUANTUM CHEMICAL STUDY OF BUTANE ISOMERIZATION ON CLUSTERS OF ALUMINUM AND COBALT CHLORIDES. MIXED COMPLEXES
RUSSIAN CHEMICAL BULLETIN 61(10), 1850-1859 (2012)
43. ZUBANOVA, EM; GOLUBEVA, EN; ZHIDOMIROV, GM.
METASTABILITY OF COPPER(II) ORGANIC COMPOUNDS: MOLECULAR DYNAMICS SIMULATION
DOKLADY PHYSICAL CHEMISTRY 446, 145-148 (2012)
44. VISHNETSKAYA, MV; IVANOVA, MS; SOLKAN, VN; ZHIDOMIROV, GM; MEL'NIKOV, MY.
ACTIVATION OF MOLECULAR OXYGEN IN TRIFLUOROACETIC ACID
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY A 86(5), 889-891 (2012)
45. LARIN, AV; RYBAKOV, AA; ZHIDOMIROV, GM.
ROLE OF DISTANT AL ATOMS IN ALKALINE EARTH ZEOLITES FOR STABILIZATION OF HYDROXYL GROUPS
JOURNAL OF PHYSICAL CHEMISTRY C 116(3), 2399-2410 (2012)
46. YULDASHEVA, GA; ZHIDOMIROV, GM; ILIN, AI.
EFFECT OF ORGANIC LIGANDS WITH CONJUGATED PI-BONDS ON THE STRUCTURE OF IODINE-ALPHA-DEXTRIN COMPLEXES
BIOTECHNOLOGY AND APPLIED BIOCHEMISTRY 59(1), 29-34 (2012)
47. ZAVELEV, DE; TSODIKOV, MV; ZHIDOMIROV, GM; KOZLOVSKII, RA.
ROLE OF THE SURFACE HYDROXYL GROUPS OF MODIFIED TITANIUM OXIDE IN CATALYTIC ETHYLENE OXIDE HYDRATION
KINETICS AND CATALYSIS 52(5), 659-671 (2011)
48. SOLKAN, VN; ZHIDOMIROV, GM.
POST-HARTREE-FOCK (MP2 AND MP4) STUDY ON DECOMPOSITION OF NITROUS OXIDE ON THE NONFRAMEWORK ALO(+) SITE IN ZSM-5 ZEOLITE
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 111(11), 2639-2648 (2011)
49. ANDRYUSHECHKIN, BV; CHERKEZ, VV; GLADCHENKO, EV; ZHIDOMIROV, GM; KIERREN, B; FAGOT-REVURAT, Y; MALTERRE, D; ELTSOV, KN.
ATOMIC STRUCTURE OF AG(111) SATURATED WITH CHLORINE: FORMATION OF AG3CL7 CLUSTERS
PHYSICAL REVIEW B 84(7), - (2011)
50. LARIN, AV; RYBAKOV, AA; ZHIDOMIROV, GM; MACE, A; LAAKSONEN, A; VERCAUTEREN, DP.
OXIDE CLUSTERS AS SOURCE OF THE THIRD OXYGEN ATOM FOR THE FORMATION OF CARBONATES IN ALKALINE EARTH DEHYDRATED ZEOLITES
JOURNAL OF CATALYSIS 281(2), 212-221 (2011)
51. GOLUBEVA, EN; GROMOV, OI; ZHIDOMIROV, GM.
CU(II)-ALKYL CHLOROCOMPLEXES: STABLE COMPOUNDS OR TRANSIENTS? DFT PREDICTION OF THEIR STRUCTURE AND EPR PARAMETERS
JOURNAL OF PHYSICAL CHEMISTRY A 115(28), 8147-8154 (2011)
52. VOLODIN, AM; MALYKHIN, SE; ZHIDOMIROV, GM.
O- RADICAL ANIONS ON OXIDE CATALYSTS: FORMATION, PROPERTIES, AND REACTIONS
KINETICS AND CATALYSIS 52(4), 605-619 (2011)
53. RYBAKOV, AA; LARIN, AV; ZHIDOMIROV, GM; TRUBNIKOV, DN; VERCAUTEREN, DP.

DFT INVESTIGATION OF CO OXIDATION OVER MG EXCHANGED PERIODIC ZEOLITE MODELS
COMPUTATIONAL AND THEORETICAL CHEMISTRY 964(1-3), 108-115 (2011)

54. KUZ'MIN, IV; SOLKAN, VN; ZHIDOMIROV, GM; KAZANSKII, VB.
MODELING OF THE MECHANISM OF ONE-ELECTRON TRANSFER FROM THE PERYLENE MOLECULE TO THE OXYGEN MOLECULE O-3(2) IN THE HF MEDIUM
KINETICS AND CATALYSIS 52(2), 192-196 (2011)

55. YULDASHEVA, GA; ZHIDOMIROV, GM; ILIN, AI.
A QUAN-TUM-CHEMICAL MODEL OF THE INHIBITION MECHANISM OF VIRAL DNA HIV-1 REPLICATION BY IODINE COMPLEX COMPOUNDS
NAT SCI 3, 573 (2011)

56. VOLODIN, A.M.; MALYHIN, S.E.; ZHIDOMIROV, G.M..
ANION-RADICALS O-ON OXIDE CATALYSTS: FORMATION, PROPERTIES AND RELATED REACTIONS
KINETICS AND CATALYSIS 52(4), 615 (2011)

57. ZHIDOMIROV, G.; SHUBIN, A. A.; LARKIN, A.; RYBAKOV, A. A.; LESZCZYNSKI, J.; SHUKLA, M. K..
MOLECULAR MODELS OF THE STABILIZATION OF BIVALENT METAL CATIONS IN ZEOLITE CATALYSTS
PUBLISHER: SPRINGER, NETHERLANDS , 579 (2011)

58. VISHNETSKAYA, MV; VASIN, AV; SOLKAN, VN; ZHIDOMIROV, GM; MEL'NIKOV, MY.
ACTIVATION OF MOLECULAR OXYGEN IN TRIFLUOROACETIC ACID
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY A 84(11), 1905-1907 (2010)

59. GLORIOZOV, IP; ZHIDOMIROV, GM; SHILINA, MI.
PROPANE TRANSFORMATIONS ON ALUMINUM CHLORIDE-COBALT CHLORIDE CLUSTERS: A QUANTUM CHEMICAL STUDY
RUSSIAN CHEMICAL BULLETIN 59(10), 1871-1880 (2010)

60. SOLKAN, VN; ZHIDOMIROV, GM; MEL'NIKOV, MY.
THE MECHANISM OF FORMATION OF THE HYDROPEROXYL RADICAL IN THE CF3COOH + O-3(2) SYSTEM: A QUANTUM-CHEMICAL STUDY
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B 4(5), 705-708 (2010)

61. ANDRYUSHECHKIN, BV; CHERKEZ, VV; GLADCHENKO, EV; ZHIDOMIROV, GM; KIERREN, B; FAGOT-REVURAT, Y; MALTERRE, D; ELTSOV, KN.
STRUCTURE OF CHLORINE ON AG(111): EVIDENCE OF THE (3X3) RECONSTRUCTION
PHYSICAL REVIEW B 81(20), - (2010)

62. LARIN, AV; RYBAKOV, AA; ZHIDOMIROV, GM; MACE, A; LAAKSONEN, A; VERCAUTEREN, DP.
THEORETICAL MODELING OF CARBONATE FORMATION IN DEHYDRATED ALKALINE EARTH ZEOLITES
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 239, - (2010)

63. LARIN, AV; ZHIDOMIROV, GM; TRUBNIKOV, DN; VERCAUTEREN, DP.
ION-EXCHANGED BINUCLEAR CA2OX CLUSTERS, X=1-4, AS ACTIVE SITES OF SELECTIVE OXIDATION OVER MOR AND FAU ZEOLITES
JOURNAL OF COMPUTATIONAL CHEMISTRY 31(2), 421-430 (2010)

64. KUZ'MIN, IV; ZHIDOMIROV, GM; SOLKAN, VN; KAZANSKII, VB.
QUANTUM CHEMICAL CALCULATION OF THE CATALYTIC REACTION OF ETHANE DEHYDROGENATION ON GALLIUM OXIDE-HYDROXIDE BINUCLEAR CLUSTERS IN OXIDIZED GAO/ZSM-5 ZEOLITE
KINETICS AND CATALYSIS 50(5), 752-759 (2009)

65. ANDRYUSHECHKIN, BV; ZHIDOMIROV, GM; ELTSOV, KN; HLADCHANKA, YV; KORLYUKOV, AA.
LOCAL STRUCTURE OF THE AG(100) SURFACE REACTING WITH MOLECULAR IODINE: EXPERIMENTAL AND THEORETICAL STUDY
PHYSICAL REVIEW B 80(12), - (2009)

66. MALYKHIN, SE; VOLODIN, AM; BEDILO, AF; ZHIDOMIROV, GM.
GENERATION OF O- RADICAL ANIONS ON MGO SURFACE: LONG-DISTANCE CHARGE SEPARATION OR HOMOLYTIC DISSOCIATION OF CHEMISORBED WATER?
JOURNAL OF PHYSICAL CHEMISTRY C 113(24), 10350-10353 (2009)

67. LARINA, AV; ZHIDOMIROV, GM; TRUBNIKOV, DN; VERCAUTEREN, DP.
DFT ANALYSIS OF PROPANE CYCLIZATION OVER BINUCLEAR GA-CLUSTERS IN MORDENITE
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 305(1-2), 90-94 (2009)

68. GOLUBEVA, EN; ZHIDOMIROV, GM; KOKORIN, AI.
ON THE STABILITY OF COPPER(II) ORGANIC COMPOUNDS WITH THE SIGMA BOND CU-C: A QUANTUM-CHEMICAL STUDY
DOKLADY CHEMISTRY 426, 143-145 (2009)

69. ZHIDOMIROV, GM; LARIN, AV; TRUBNIKOV, DN; VERCAUTEREN, DP.
ION-EXCHANGED BINUCLEAR CLUSTERS AS ACTIVE SITES OF SELECTIVE OXIDATION OVER ZEOLITES
JOURNAL OF PHYSICAL CHEMISTRY C 113(19), 8258-8265 (2009)
70. ZHANPEISOV, NU; ZHIDOMIROV, GM; FUKUMURA, H.
INTERACTION OF A SINGLE WATER MOLECULE WITH A SINGLE GRAPHITE LAYER: AN INTEGRATED ONIOM STUDY
JOURNAL OF PHYSICAL CHEMISTRY C 113(15), 6118-6123 (2009)
71. SOLKAN, VN; ZHIDOMIROV, GM.
MP2 STUDY ON DECOMPOSITION OF NITROUS OXIDE ON THE GA-ZSM-5
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 108(14), 2732-2743 (2008)
72. PIDKO, EA; HENSEN, EJM; ZHIDOMIROV, GM; VAN SANTEN, RA.
NON-LOCALIZED CHARGE COMPENSATION IN ZEOLITES: A PERIODIC DFT STUDY OF CATIONIC GALLIUM-OXIDE CLUSTERS IN MORDENITE
JOURNAL OF CATALYSIS 255(2), 139-143 (2008)
73. ZHIDOMIROV, GM; SHUBIN, AA; MILOV, MA; KAZANSKY, VB; VAN SANTEN, RA; HENSEN, EJM.
CLUSTER MODEL DFT STUDY OF CO ADSORPTION TO GALLIUM IONS IN GA/HZSM-5
JOURNAL OF PHYSICAL CHEMISTRY C 112(9), 3321-3326 (2008)
74. MALYKHIN, SE; VOLODIN, AM; ZHIDOMIROV, GM.
SPIN STATES OF IRON-NITROSYL ADSORPTION COMPLEXES FORMED IN FE-ZSM5 ZEOLITES
APPLIED MAGNETIC RESONANCE 33(1-2), 153-166 (2008)
75. SUBBOTINA, IR; SOKOLOVA, NA; KUZ'MIN, IV; SHUBIN, AA; ZHIDOMIROV, GM; KAZANSKII, VB.
ADSORPTION PROPERTIES OF OXIDIZED GALLIUM-MODIFIED ZEOLITE ZSM-5 FROM DIFFUSE-REFLECTANCE IR-SPECTROSCOPIC AND QUANTUM-CHEMICAL DATA: II. INTERACTION WITH CARBON MONOXIDE AND WATER
KINETICS AND CATALYSIS 49(1), 149-155 (2008)
76. AVDEEV, VI; KOVALCHUK, VI; ZHIDOMIROV, GM; D'ITRI, JL.
MODELS OF ACTIVE SITES IN SUPPORTED CU METAL CATALYSTS IN 1,2-DICHLOROETHANE DECHLORINATION. DFT ANALYSIS
JOURNAL OF STRUCTURAL CHEMISTRY 48, S160-S170 (2007)
77. AVDEEV, VI; KOVALCHUK, VI; ZHIDOMIROV, GM; D'ITRI, JL.
DFT ANALYSIS OF THE MECHANISM OF 1,2-DICHLOROETHANE DECHLORINATION ON SUPPORTED CU-PT BIMETALLIC CATALYSTS
JOURNAL OF STRUCTURAL CHEMISTRY 48, S171-S183 (2007)
78. SOLKAN, VN; ZHIDOMIROV, GM; KAZANSKY, VB.
DENSITY FUNCTIONAL THEORY STUDIES OF NITROUS OXIDE ADSORPTION AND DECOMPOSITION ON GA-ZSM-5
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 107(13), 2417-2425 (2007)
79. KUSMIN, IV; ZHIDOMIROV, GM; SOLKAN, VN.
SWIFT HOPPING GALLIUM OVER [ALO4](-) SWIFT TETRAHEDRA IN GA/ZSM-5: A DFT STUDY
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 107(13), 2434-2441 (2007)
80. YULDASHEVA, G; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL EXAMINATION OF INTERACTION OF CYTOSTATIC-FLUOROURACIL WITH DEOXYRIBONUCLEIC ACIDS
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 107(13), 2384-2388 (2007)
81. MALYKHIN, SE; ANUFRIENKO, VF; HANSEN, EJM; KUZNETSOVA, EV; LARINA, TV; ZHIDOMIROV, GM.
DISTORTION OF THE TETRAHEDRAL COORDINATION OF FE(III) IONS STABILIZED IN ZSM-5 ZEOLITE FRAMEWORK
JOURNAL OF STRUCTURAL CHEMISTRY 48(5), 855-861 (2007)
82. SUBBOTINA, IR; SOKOLOVA, NA; KUZ'MIN, IV; ZHIDOMIROV, GM; KAZANSKII, VB.
ADSORPTION PROPERTIES OF OXIDIZED GALLIUM-MODIFIED ZEOLITE ZSM-5 FROM DIFFUSE REFLECTANCE IR AND QUANTUM-CHEMICAL DATA: 1. INTERACTION WITH HYDROGEN AND ETHANE
KINETICS AND CATALYSIS 48(5), 735-741 (2007)
83. KUZ'MIN, I. V.; ZHIDOMIROV, G. M.; SOLKAN, V. N..
STABILITY AND CHEMICAL ACTIVITY OF BINUCLEAR GALLIUM OXIDE CLUSTERS IN GAO/ZSM-5
CONFERENCE: PROC.OF THE 18TH MENDELEEV CONF. ON GENERAL AND APPLIED CHEMISTRY LOCATION: MOSCOW 3, 379 (2007)
84. KUZMIN, IV; ZHIDOMIROV, GM; HENSEN, EJM.
A DFT STUDY OF HYDROGEN-DEUTERIUM EXCHANGE OVER OXIDIZED AND REDUCED GALLIUM SPECIES IN GA/HZSM-5 ZEOLITE
CATALYSIS LETTERS 108(3-4), 187-191 (2006)

85. LAPIDUS, AL; MIKHAILOV, MN; DERGACHEV, AA; ZHIDOMIROV, GM; MISHIN, IV.
THE NATURE OF ACTIVE SITES IN PT PROMOTED GAZSM-5 CATALYSTS
REACTION KINETICS AND CATALYSIS LETTERS 87(2), 249-254 (2006)
86. VOLODIN, AM; ZHIDOMIROV, GM; DUBKOV, KA; HENSEN, EJM; VAN SANTEN, RA.
SPIN DESIGN OF IRON COMPLEXES ON FE-ZSM-5 ZEOLITES
CATALYSIS TODAY 110(3-4), 247-254 (2005)
87. MALYKHIN, S; ZILBERBERG, I; ZHIDOMIROV, GM.
ELECTRON STRUCTURE OF OXYGEN COMPLEXES OF FERROUS ION CENTER
CHEMICAL PHYSICS LETTERS 414(4-6), 434-437 (2005)
88. MIKHAILOV, MN; ZHIDOMIROV, GM; KRYLOVA, AY.
INTERACTION OF CO-6 CLUSTER WITH GAMMA-ALUMINA SURFACE: A QUANTUM CHEMICAL STUDY
RUSSIAN CHEMICAL BULLETIN 54(10), 2264-2269 (2005)
89. ZHIDOMIROV, GM; SHUBIN, AA; KAZANSKY, VB; VAN SANTEN, RA.
SPECTROSCOPIC IDENTIFICATION OF ADSORPTION PROPERTIES OF ZN2+ IONS AT CATIONIC POSITIONS OF HIGH-SILICA ZEOLITES WITH DISTANT PLACING OF ALUMINIUM IONS
THEORETICAL CHEMISTRY ACCOUNTS 114(1-3), 90-96 (2005)
90. AVDEEV, VI; ZHIDOMIROV, GM.
MODELING THE ACTIVE CENTERS OF V2O5/SIO2 AND V2O5/TIO2 SUPPORTED CATALYSTS. DFT THEORETICAL ANALYSIS OF OPTICAL PROPERTIES
JOURNAL OF STRUCTURAL CHEMISTRY 46(4), 577-590 (2005)
91. AVDEEV, VI; KOVALCHUK, VI; ZHIDOMIROV, GM; D'ITRI, JL.
ETHYLENE ADSORPTION ON THE PT-CU BIMETALLIC CATALYSTS. DENSITY FUNCTIONAL THEORY CLUSTER STUDY
SURFACE SCIENCE 583(1), 46-59 (2005)
92. AVDEEV, VI; RUZANKIN, SF; ZHIDOMIROV, GM.
MOLECULAR MECHANISM OF DIRECT ALKENE OXIDATION WITH NITROUS OXIDE: DFT ANALYSIS
KINETICS AND CATALYSIS 46(2), 177-188 (2005)
93. BEDILO, AF; PLOTNIKOV, MA; MEZENTSEVA, NV; VOLODIN, AM; ZHIDOMIROV, GM; RYBKIN, IM; KLABUNDE, KJ.
SUPEROXIDE RADICAL ANIONS ON THE SURFACE OF ZIRCONIA AND SULFATED ZIRCONIA: FORMATION MECHANISMS, PROPERTIES AND STRUCTURE
PHYSICAL CHEMISTRY CHEMICAL PHYSICS 7(16), 3059-3069 (2005)
94. AVDEEV, V.I.; RUZANKIN, S.F.; ZHIDOMIROV, G.M..
MOLECULAR MECHANISM OF DIRECT ALKENE OXIDATION BY NITROUS OXIDE: DFT ANALYSIS
KINETIKA I KATALIZ 46(2), 191 (2005)
95. MILCHAFLOV, M. N.; ZHIDOMIROV, G. M.; KRYLOVA, A. Y..
INTERACTION OF COB CLUSTER WITH Y-ALUMINA SURFACE: A QUANTUM CHEMICAL STUDY
RUSS. CHEM. BULL. 54, 2264 (2005)
96. ZHIDOMIROV, GM; SHUBIN, AA; VAN SANTEN, RA; CATLOW, CRA; VAN SANTEN, RA; SMIT, B.
STRUCTURE AND REACTIVITY OF METAL ION SPECIES IN HIGH-SILICA ZEOLITES
PUBLISHER: WILEY, VERLAG , 201 (2005); ELSEVIER, AMSTERDAM, NETHERLANDS , 201 (2004)…
97. ZHIDOMIROV, GM; SHUBIN, AA; KAZANSKY, VB; VAN SANTEN, RA.
POSSIBLE MOLECULAR STRUCTURE OF PROMOTED LEWIS ACIDITY SITES IN ZNZSM-5
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 100(4), 489-494 (2004)
98. ZILBERBERG, I; RUZANKIN, SP; MALYKHIN, S; ZHIDOMIROV, GM.
UNRESTRICTED DENSITY FUNCTIONAL THEORY OF THE BONDING BETWEEN NO RADICAL AND FERROUS ION
CHEMICAL PHYSICS LETTERS 394(4-6), 392-396 (2004)
99. FROLOVA, YV; AVDEEV, VI; RUZANKIN, SP; ZHIDOMIROV, GM; FEDOTOV, MA; SADYKOV, VA.
EXPERIMENTAL AND THEORETICAL STUDIES OF THE ELECTRONIC SPECTRA OF MIXED FRAMEWORK PHOSPHATES OF ZR AND CO
JOURNAL OF PHYSICAL CHEMISTRY B 108(22), 6969-6980 (2004)
100. KOSHELEVA, AS; YUDANOV, IV; ZHIDOMIROV, GM; PARMON, VN.
COPPER HYDROXIDE CATALYSTS FOR SELECTIVE OXIDATION: QUANTUM CHEMICAL STUDY OF ACTIVE SITES
REACTION KINETICS AND CATALYSIS LETTERS 82(2), 347-354 (2004)
101. AVDEEV, VI; ZHIDOMIROV, GM.
MODELS OF FINELY DISPERSED MGO AND V2O5 ON SILICA. THEORETICAL ANALYSIS OF OPTICAL PROPERTIES USING TDDFT
RESEARCH ON CHEMICAL INTERMEDIATES 30(1), 41-64 (2004)
102. RUZANKIN, SP; ZILBERBERG, I; ZHIDOMIROV, GM.

CLOSED AND OPEN-SHELL ATOMIC OXYGEN ON SILVER: TWO DISTINCT PATTERNS OF THE O-1S BINDING ENERGY AND X-RAY ABSORPTION 0 K-EDGE SPECTRA AS REVEALED BY DENSITY FUNCTIONAL THEORY
RESEARCH ON CHEMICAL INTERMEDIATES 30(1), 75-85 (2004)

103. KACHUROVSKAYA, NA; ZHIDOMIROV, GM; VAN SANTEN, RA.
COMPARATIVE ENERGIES OF ZN(II) CATION LOCALIZATION AS A FUNCTION OF THE DISTANCE BETWEEN TWO FORMING CATION POSITION ALUMINIUM IONS IN HIGH-SILICA ZEOLITES
RESEARCH ON CHEMICAL INTERMEDIATES 30(1), 99-103 (2004)

104. PATRAKOV, AE; GRITSENKO, VA; ZHIDOMIROV, GM.
INTERACTION WITH CHARGE CARRIERS AND THE OPTICAL ABSORPTION SPECTRUM OF AN ASSOCIATE FORMED BY ELEMENTARY DEFECTS (AN OXYGEN VACANCY AND A SILYLENE CENTER) IN SIO2
PHYSICS OF THE SOLID STATE 46(11), 2021-2025 (2004)

105. AVDEEV, VI; ZHIDOMIROV, GM.
ELECTRONIC STRUCTURE AND OPTICAL PROPERTIES OF THE SURFACE F-CENTERS IN MGO: A THEORETICAL ANALYSIS BY DFT APPROACH
JOURNAL OF STRUCTURAL CHEMISTRY 44(6), 918-926 (2003)

106. SHUBIN, AA; ZHIDOMIROV, GM; KAZANSKY, VB; VAN SANTEN, RA.
DFT CLUSTER MODELING OF MOLECULAR AND DISSOCIATIVE HYDROGEN ADSORPTION ON ZN2+ IONS WITH DISTANT PLACING OF ALUMINUM IN THE FRAMEWORK OF HIGH-SILICA ZEOLITES
CATALYSIS LETTERS 90(3-4), 137-142 (2003)

107. BOROVKOV, VY; MIKHEEVA, EP; ZHIDOMIROV, GM; LAPINA, OB.
THEORETICAL AND EXPERIMENTAL STUDIES OF THE NATURE OF THE CATALYTIC ACTIVITY OF VOX/TIO2 SYSTEMS
KINETICS AND CATALYSIS 44(5), 710-717 (2003)

108. RUZANKIN, SF; AVDEEV, VI; DOBRYNKIN, NM; ZHIDOMIROV, GM; NOSKOV, AS.
MODELING ACTIVE CENTERS IN AMMONIA SYNTHESIS. DFT STUDY OF DISSOCIATIVE ADSORPTION OF N-2 ON RU CLUSTERS
JOURNAL OF STRUCTURAL CHEMISTRY 44(3), 341-350 (2003)

109. GRITSENKO, VA; SHAPOSHNIKOV, AV; NOVIKOV, YN; BARABAN, AP; WONG, H; ZHIDOMIROV, GM; ROGER, M.
ONEFOLD COORDINATED OXYGEN ATOM: AN ELECTRON TRAP IN THE SILICON OXIDE
MICROELECTRONICS RELIABILITY 43(4), 665-669 (2003)

110. KACHUROVSKAYA, NA; ZHIDOMIROV, GM; HENSEN, EJM; VAN SANTEN, RA.
CLUSTER MODEL DFT STUDY OF THE INTERMEDIATES OF BENZENE TO PHENOL OXIDATION BY N2O ON FEZSM-5 ZEOLITES
CATALYSIS LETTERS 86(1-3), 25-31 (2003)

111. AVDEEV, VI; RUZANKIN, SP; ZHIDOMIROV, GM.
MECHANISM OF DIRECT OXIDATION OF CYCLOHEXENE TO CYCLOHEXANONE WITH NITROUS OXIDE. THEORETICAL ANALYSIS BY DFT METHOD
CHEMICAL COMMUNICATIONS (1), 42-43 (2003)

112. GRITSENKO, VA; NOVIKOV, YN; SHAPOSHNIKOV, AV; WONG, H; ZHIDOMIROV, GM.
CAPTURING PROPERTIES OF A THREEFOLD COORDINATED SILICON ATOM IN SILICON NITRIDE: POSITIVE CORRELATION ENERGY MODEL
PHYSICS OF THE SOLID STATE 45(11), 2031-2035 (2003)

113. ZHIDOMIROV, GM; AVDEEV, VI; BORONIN, AI.
MOLECULAR MECHANISM OF ETHYLENE EPOXIDATION ON SILVER: STATE OF THE PROBLEM AND THEORETICAL APPROACHES
COMPUTATIONAL MATERIALS SCIENCE 187, 334-358 (2003)

114. ZILBERBERG, I; GORA, RW; ZHIDOMIROV, GM; LESZCZYNSKI, J.
BONDING IN THE OXO FERROUS IRON SPECIES: A COMPLETE ACTIVE-SPACE SELF-CONSISTENT-FIELD THEORY VERIFICATION OF THE MOLECULAR-OXYGEN-LIKE PATTERN
JOURNAL OF CHEMICAL PHYSICS 117(15), 7153-7161 (2002)

115. KACHUROVSKAYA, NA; ZHIDOMIROV, GM; MINOT, C.
PERIODIC DFT STUDY OF ISOMORPHOUS INCORPORATION OF A V ION INTO (100) AND (001) ANATASE SURFACE LAYERS
SURFACE REVIEW AND LETTERS 9(3-4), 1425-1430 (2002)

116. SHAPOSHNIKOV, AV; GRITSENKO, VA; ZHIDOMIROV, GM; ROGER, M.
HOLE TRAPPING ON THE TWOFOLD-COORDINATED SILICON ATOM IN SIO2
PHYSICS OF THE SOLID STATE 44(6), 1028-1030 (2002)

117. RUZANKIN, SF; SHVEIGERT, IV; ZHIDOMIROV, GM.
NEST DEFECT AS THE SITE OF STABILIZATION OF TRANSITION ELEMENT IONS IMPLANTED IN HIGH-SILICA ZEOLITES. CLUSTER CALCULATION OF FE(II) AND FE(III) IONS ENTRAPPED BY THE ZEOLITE MATRIX
JOURNAL OF STRUCTURAL CHEMISTRY 43(2), 229-233 (2002)
118. MIKHEEVA, EP; KACHUROVSKAYA, NA; ZHIDOMIROV, GM.
CLUSTER MODELS OF THE VOX/TIO2 SUPPORTED CATALYST
KINETICS AND CATALYSIS 43(2), 223-232 (2002)
119. KIRILLOV, MA; ZHIDOMIROV, GM.
CLUSTER MODELS OF CO2+ AT THE CATION SITES OF ZEOLITE ZSM-5
JOURNAL OF STRUCTURAL CHEMISTRY 43(2), 225-228 (2002)
120. KACHUROVSKAYA, NA; MIKHEEVA, EP; ZHIDOMIROV, GM.
CLUSTER MOLECULAR MODELING OF STRONG INTERACTION FOR VOX/TIO2 SUPPORTED CATALYST
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 178(1-2), 191-198 (2002)
121. GRITSENKO, VA; SHAPOSHNIKOV, A; ZHIDOMIROV, GM; ROGER, M.
TWO FOLD COORDINATED SILICON ATOM: A HOLE TRAP IN SIO2
SOLID STATE COMMUNICATIONS 121(6-7), 301-304 (2002)
122. AVDEEV, VI; BORONIN, AI; ZHIDOMIROV, GM.
PROPERTIES OF ADSORBED OXYGEN FORMS ON A DEFECTIVE AG(111) SURFACE. DFT ANALYSIS
JOURNAL OF STRUCTURAL CHEMISTRY 43(1), 26-32 (2002)
123. MILOV, MA; ZHIDOMIROV, GM.
DFT CLUSTER MODEL OF HYDROPEROXIDE ACTIVATION INTERMEDIATES IN TI-CONTAINING POROUS SILICATES
REACTION KINETICS AND CATALYSIS LETTERS 75(1), 147-155 (2002)
124. GRITSENKO, VA; SHAPOSHNIKOV, AV; NOVIKOV, YN; BARABAN, AP; HEI, W; ZHIDOMIROV, GM; ROGER, M.
NUMERICAL STUDY OF ONE-FOLD COORDINATED OXYGEN ATOM IN SILICON GATE OXIDE
2002 IEEE HONG KONG ELECTRON DEVICES MEETING, PROCEEDINGS , 39-42 (2002)
125. YAKOVLEV, AL; ZHIDOMIROV, GM; VAN SANTEN, RA.
DFT CALCULATIONS ON N2O DECOMPOSITION BY BINUCLEAR FE COMPLEXES IN FE/ZSM-5
JOURNAL OF PHYSICAL CHEMISTRY B 105(49), 12297-12302 (2001)
126. AVDEEV, VI; ZHIDOMIROV, GM.
ETHYLENE AND OXYGEN SPECIES ADSORBED ON A DEFECT OXIDIZED SURFACE AG(111) - THEORETICAL ANALYSIS BY DFT METHOD
SURFACE SCIENCE 492(1-2), 137-151 (2001)
127. SHUBIN, AA; ZHIDOMIROV, GM; YAKOVLEV, AL; VAN SANTEN, RA.
COMPARATIVE QUANTUM CHEMICAL STUDY OF STABILIZATION ENERGIES OF ZN2+ IONS IN DIFFERENT ZEOLITE STRUCTURES
JOURNAL OF PHYSICAL CHEMISTRY B 105(21), 4928-4935 (2001)
128. BARBOSA, LAMM; ZHIDOMIROV, GM; VAN SANTEN, RA.
THEORETICAL STUDY OF THE MOLECULAR HYDROGEN ADSORPTION AND DISSOCIATION ON DIFFERENT ZN(II) ACTIVE SITES OF ZEOLITES
CATALYSIS LETTERS 77(1-3), 55-62 (2001)
129. YAKOVLEV, AL; ZHIDOMIROV, GM; VAN SANTEN, RA.
N2O DECOMPOSITION CATALYSED BY TRANSITION METAL IONS
CATALYSIS LETTERS 75(1-2), 45-48 (2001)
130. VAN SANTEN, RA; ZHIDOMIROV, GM; SHUBIN, AA; YAKOVLEV, AL; BARBOSA, LAMM.
REACTIVITY THEORY OF ZINC CATION SPECIES IN ZEOLITES
CATALYSIS BY UNIQUE METAL ION STRUCTURES IN SOLID MATRICES: FROM SCIENCE TO APPLICATION 13, 187-204 (2001)
131. BORONIN, AI; KOSCHEEV, SV; MURZAKHMETOV, KT; AVDEEV, VI; ZHIDOMIROV, GM.
ASSOCIATIVE OXYGEN SPECIES ON THE OXIDIZED SILVER SURFACE FORMED UNDER O-2 MICROWAVE EXCITATION
APPLIED SURFACE SCIENCE 165(1), 9-14 (2000)
132. KACHUROVSKAYA, NA; ZHIDOMIROV, GM; ARISTOV, YI.
ON THE PROBLEM OF DIFFERENTIATION OF ACETONE ADSORPTION SPECIES ON THE SILICA GEL: MOLECULAR MODELS OF ADSORPTION COMPLEXES
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 158(1), 281-285 (2000)
133. MILOV, MA; ZILBERBERG, IL; RUZANKIN, SP; ZHIDOMIROV, GM.
OXYGEN ADSORPTION ON THE AG(111) SURFACE: A QUANTUM CHEMICAL STUDY BY THE NDDO/MC METHOD

JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 158(1), 309-312 (2000)

134. ZHIDOMIROV, GM; PARMON, VN.
SPECIAL ISSUE - PHYSICAL METHODS FOR CATALYTIC RESEARCH AT THE MOLECULAR LEVEL: DEDICATED TO THE MEMORY OF PROFESSOR K.I. ZAMARAEV - PREFACE
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 158(1), 1-3 (2000)

135. ELIZAROVA, GL; ZHIDOMIROV, GM; PARMON, VN.
HYDROXIDES OF TRANSITION METALS AS ARTIFICIAL CATALYSTS FOR OXIDATION OF WATER TO DIOXYGEN
CATALYSIS TODAY 58(2-3), 71-88 (2000)

136. AVDEEV, VI; BORONIN, AI; KOSCHEEV, SV; ZHIDOMIROV, GM.
QUASIMOLECULAR STABLE FORMS OF OXYGEN ON SILVER SURFACE. THEORETICAL ANALYSIS BY THE DENSITY FUNCTIONAL THEORY METHOD
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 154(1-2), 257-270 (2000)

137. TYUPALO, NF; ZAKHAROV, II; KOLBASINA, OI; ZHIDOMIROV, GM; AVDEEV, VI.
DENSITY FUNCTIONAL CALCULATION FOR OZONE-ETHYLENE COMPLEXES
JOURNAL OF STRUCTURAL CHEMISTRY 41(2), 194-199 (2000)

138. MILOV, MA; ZILBERBERG, IL; RUZANKIN, SF; ZHIDOMIROV, GM.
OXYGEN DIFFUSION THROUGH THE AG(111) SURFACE: A QUANTUM CHEMICAL STUDY BY THE NDDO/MC METHOD
JOURNAL OF STRUCTURAL CHEMISTRY 41(2), 200-205 (2000)

139. YAKOVLEV, AL; SHUBIN, AA; ZHIDOMIROV, GM; VAN SANTEN, RA.
DFT STUDY OF OXYGEN-BRIDGED ZN2+ ION PAIRS IN ZN/ZSM-5 ZEOLITES
CATALYSIS LETTERS 70(3-4), 175-181 (2000)

140. BARBOSA, LAMM; ZHIDOMIROV, GM; VAN SANTEN, RA.
THEORETICAL STUDY OF METHANE ADSORPTION ON ZN(II) ZEOLITES
PHYSICAL CHEMISTRY CHEMICAL PHYSICS 2(17), 3909-3918 (2000)

141. BORONIN, AI; AVDEEV, VI; KOSHCHEEV, SV; MURZAKHMETOV, KT; RUZANKIN, SF; ZHIDOMIROV, GM.
THE CONCEPT OF QUASIMOLECULAR ELECTROPHILIC OXYGEN IN ETHYLENE EPOXIDATION OVER SILVER
KINETICS AND CATALYSIS 40(5), 653-672 (1999)

142. ZHIDOMIROV, GM; YAKOVLEV, AL; MILOV, MA; KACHUROVSKAYA, NA; YUDANOV, IV.
MOLECULAR MODELS OF CATALYTICALLY ACTIVE SITES IN ZEOLITES. QUANTUM CHEMICAL APPROACH
CATALYSIS TODAY 51(3-4), 397-410 (1999)

143. AVDEEV, VI; ZHIDOMIROV, GM.
ATOMIC AND MOLECULAR FORMS OF OXYGEN ON AG(331). THEORETICAL ANALYSIS USING THE DFT METHOD
JOURNAL OF STRUCTURAL CHEMISTRY 40(3), 343-349 (1999)

144. ZILBERBERG, IL; MILOV, MA; ZHIDOMIROV, GM.
FORMS OF CHEMISORBED OXYGEN ON AG(111): NDDO/MC SEMIEMPIRICAL INVESTIGATION
JOURNAL OF STRUCTURAL CHEMISTRY 40(3), 350-357 (1999)

145. ZAKHAROV, II; ZAKHAROV, VA; POTAPOV, AG; ZHIDOMIROV, GM.
A DFT QUANTUM-CHEMICAL STUDY ON THE STRUCTURES AND ACTIVE SITES OF POLYMETHYLALUMINOXANE
MACROMOLECULAR THEORY AND SIMULATIONS 8(3), 272-278 (1999)

146. IVANOV, EA; BORONIN, AI; KOSCHEEV, SV; ZHIDOMIROV, GM.
MODELING OF OXYGEN ADSORPTION ON SILVER
REACTION KINETICS AND CATALYSIS LETTERS 66(2), 265-272 (1999)

147. ZILBERBERG, IL; ZHIDOMIROV, GM.
SEMIEMPIRICAL NDDO/MC CALCULATIONS OF THE EXCITED STATES OF THE CHROMATE ION
JOURNAL OF STRUCTURAL CHEMISTRY 40(2), 187-191 (1999)

148. ZAKHAROV, II; STARTSEV, AN; ZHIDOMIROV, GM; PARMON, VN.
OXIDATIVE ADDITION OF DIHYDROGEN AS THE KEY STEP OF THE ACTIVE CENTER FORMATION IN THE HDS SULFIDE BIMETALLIC CATALYSTS: AB INITIO MO/MP2 STUDY
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 137(1-3), 101-111 (1999)

149. YAKOVLEV, AL; ZHIDOMIROV, GM.
QUANTUM CHEMICAL STUDY OF NITROUS OXIDE ADSORPTION AND DECOMPOSITION ON LEWIS ACID SITES
CATALYSIS LETTERS 63(1-2), 91-95 (1999)

150. ZILBERBERG, IL; MILOV, MA; ZHIDOMIROV, GM.
SCALING THE COULOMB INTERACTION IN CALCULATIONS OF ELECTRON SPECTRA OF TRANSITION METAL COMPLEXES
JOURNAL OF STRUCTURAL CHEMISTRY 40(1), 1-9 (1999)

151. BORONIN, AI; KOSCHEEV, SV; ZHIDOMIROV, GM.
XPS AND UPS STUDY OF OXYGEN STATES ON SILVER
JOURNAL OF ELECTRON SPECTROSCOPY AND RELATED PHENOMENA 96(1-3), 43-51 (1998)
152. VOLODIN, AM; SOBOLEV, VI; ZHIDOMIROV, GM.
THE IN SITU ESR STUDY OF THE STATE OF IRON IONS IN FE-ZSM-5 ZEOLITES
KINETICS AND CATALYSIS 39(6), 775-787 (1998)
153. AVDEEV, VI; ZHIDOMIROV, GM.
ADDUCTS OF HYDROGEN AND METHANE WITH OS(II) AND OS(IV) COMPLEXES: THEORETICAL ANALYSIS OF (ETA(2)-H-2)OSCL2(PH3)(2) AND (ETA-CH4)OSCL2(PH3)(2) MOLECULAR COMPLEXES BY RHF, MP2 AND DFT METHODS
CATALYSIS TODAY 42(3), 247-261 (1998)
154. AVDEEV, VI; ZHIDOMIROV, GM.
METHANE ACTIVATION BY OS(II) COMPLEXES: THEORETICAL STUDY OF METHANE OXIDATIVE ADDITION TO ISOMERIC OSCL2(PH3)(2) COMPLEXES BY RHF, MP2, AND DFT METHODS
KINETICS AND CATALYSIS 39(4), 476-484 (1998)
155. ZAKHAROV, II; STARTSEV, AN; ZHIDOMIROV, GM.
OXIDATIVE ADDITION OF DIHYDROGEN TO NI(II) COMPLEXES. AB INITIO MO/MP4 CALCULATIONS OF THE ELECTRONIC STRUCTURE OF NIH2CL2(PH-3)(2) COMPLEX
REACTION KINETICS AND CATALYSIS LETTERS 64(2), 247-254 (1998)
156. MIKHEEVA, EP; KOSCHEEV, SV; RUZANKIN, SP; ZHIDOMIROV, GM; LEONTIEV, SA; DEVJATOV, VG; CHERKASHIN, AE.
AN EFFECT OF THE ZN3D-STATES ON UV AND X-RAY SPECTRA IN ZNO
JOURNAL OF ELECTRON SPECTROSCOPY AND RELATED PHENOMENA 94(1-2), 59-71 (1998)
157. BORONIN, AI; KOSCHEEV, SV; KALINKINA, OV; ZHIDOMIROV, GM.
OXYGEN STATES DURING THERMAL DECOMPOSITION OF AG2O: XPS AND UPS STUDY
REACTION KINETICS AND CATALYSIS LETTERS 63(2), 291-296 (1998)
158. ZILBERBERG, IL; AVDEEV, VI; ZHIDOMIROV, GM.
EFFECT OF CISPLATIN BINDING ON GUANINE IN NUCLEIC ACID: AN AB INITIO STUDY
THEOCHEM-JOURNAL OF MOLECULAR STRUCTURE 418(1), 73-81 (1997)
159. MIKHEEVA, EP; ZHIDOMIROV, GM; RUZANKIN, SF; LEONTIEV, SA; DEVYATOV, VG; KOSHCHEEV, SV; CHERKASHIN, AE.
MODELING THE PHOTOELECTRON SPECTRA OF THE VALENCE O2P-BAND OF ZINC OXIDE BY THE XA-SCATTERED WAVE METHOD
JOURNAL OF STRUCTURAL CHEMISTRY 38(5), 732-741 (1997)
160. MILOV, MA; RUZANKIN, SF; ZHIDOMIROV, GM.
ON THE MOLECULAR MODELS OF LEWIS ACID SITES ON THE SURFACE OF GAMMA-AL2O3 AND IN ZEOLITES: A DENSITY FUNCTIONAL STUDY OF CO ADSORPTION
JOURNAL OF STRUCTURAL CHEMISTRY 38(5), 698-702 (1997)
161. AVDEEV, VI; RUZANKIN, SF; ZHIDOMIROV, GM.
THEORETICAL ANALYSIS OF THERMALLY STABLE ADSORPTION FORMS OF OXYGEN ON SILVER
JOURNAL OF STRUCTURAL CHEMISTRY 38(4), 519-527 (1997)
162. ZILBERBERG, IL; ZHIDOMIROV, GM.
FORMS OF CHEMISORBED OXYGEN ON AG(110): SEMIEMPIRICAL INVESTIGATION BY THE NDDO/MC METHOD
JOURNAL OF STRUCTURAL CHEMISTRY 38(4), 528-535 (1997)
163. ZAKHAROV, II; STARTSEV, AN; ZHIDOMIROV, GM.
QUANTUM CHEMICAL STUDY OF THE ELECTRONIC STRUCTURE OF THE NI/MOS2 HYDRODESULFURIZATION CATALYSTS
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 119(1-3), 437-447 (1997)
164. YUDANOV, IV; ZAKHAROV, II; STARTSEV, AN; ZHIDOMIROV, GM.
CHELATE COMPLEX NI(S2C2H2)(2) AS A MOLECULAR MODEL OF THE HYDRODESULFURIZATION ACTIVE CENTER
REACTION KINETICS AND CATALYSIS LETTERS 61(1), 117-122 (1997)
165. ZAKHAROV, II; ZAKHAROV, VA; ZHIDOMIROV, GM.
AB INITIO CALCULATIONS OF PROPYLENE ADDITION TO THE METAL-METHYL BOND IN TITANIUM AND ALUMINUM ALKYL COMPLEXES
KINETICS AND CATALYSIS 38(2), 231-235 (1997)
166. TAPILIN, VM; ZHIDOMIROV, GM.
EXACT CALCULATION OF THE CURRENT IN A ONE-DIMENSION MODEL OF A SCANNING TUNNELING

MICROSCOPE
SURFACE SCIENCE 370(2-3), 259-267 (1997)

167. BORONIN, AI; KOSCHEEV, SV; MALAKHOV, VF; ZHIDOMIROV, GM.
STUDY OF HIGH-TEMPERATURE OXYGEN STATES ON THE SILVER SURFACE BY XPS AND UPS
CATALYSIS LETTERS 47(2), 111-117 (1997)

168. AVDEEV, VI; ZHIDOMIROV, GM.
METHANE OXIDATIVE ADDITION TO PT(CL)(2)(PH3)(2) AND PT(CL)(2)(PH3) COMPLEXES
KINETICS AND CATALYSIS 37(5), 722-731 (1996)

169. ZAKHAROV, II; ZAKHAROV, VA; ZHIDOMIROV, GM.
QUANTUM CHEMICAL STUDIES OF PROPENE, ETHYLENE, ACETYLENE AND DIHYDROGEN REACTIVITY IN THE INSERTION REACTION INTO THE TITANIUM-ALKYL BOND
MACROMOLECULAR THEORY AND SIMULATIONS 5(5), 837-843 (1996)

170. ZHIDOMIROV, GM; ZHANPEISOV, NU; ZILBERBERG, IL; YUDANOV, IV.
ON SOME WAYS OF MODIFYING SEMIEMPIRICAL QUANTUM CHEMICAL METHODS
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 58(2), 175-184 (1996)

171. YAKOVLEV, AL; ZHIDOMIROV, GM; NEYMAN, KM; NASLUZOV, VA; ROSCH, N.
ELECTRON-DEFICIENT PALLADIUM CLUSTERS IN ZEOLITES AND THEIR COMPLEXES WITH PROBE CO MOLECULES. A DENSITY FUNCTIONAL MODEL CLUSTER STUDY
BERICHTE DER BUNSEN-GESELLSCHAFT-PHYSICAL CHEMISTRY CHEMICAL PHYSICS 100(4), 413-417 (1996)

172. ZAKHAROV, II; STARTSEV, AN; YUDANOV, IV; ZHIDOMIROV, GM.
AB INITIO QUANTUM CHEMICAL CALCULATION OF THE ELECTRONIC STRUCTURE OF THE CHELATE COMPLEX NI(S2C2H2)(2)
JOURNAL OF STRUCTURAL CHEMISTRY 37(2), 201-205 (1996)

173. ZHIDOMIROV, GM; ARBUZNIKOV, AV; YUDANOV, IV; KACHUROVSKAYA, NA.
QUANTUM CHEMICAL TREATMENT OF ACTIVE SITES IN ZEOLITES
REACTION KINETICS AND CATALYSIS LETTERS 57(2), 263-274 (1996)

174. YAKOVLEV, AL; NEYMAN, KM; ZHIDOMIROV, GM; ROSCH, N.
INTERACTION OF CO MOLECULES WITH ELECTRON-DEFICIENT PT ATOMS IN ZEOLITES: A DENSITY FUNCTIONAL MODEL CLUSTER STUDY
JOURNAL OF PHYSICAL CHEMISTRY 100(9), 3482-3487 (1996)

175. ARBUZNIKOV, AV; ZHIDOMIROV, GM.
SELECTIVE OXIDATION OF METHANE BY DINITROGEN MONOXIDE ON FEZSM-5 ZEOLITES. AB INITIO QUANTUM CHEMICAL ANALYSIS
CATALYSIS LETTERS 40(1-2), 17-23 (1996)

176. NEYMAN, KM; NASLUZOV, VA; ZHIDOMIROV, GM.
A DENSITY FUNCTIONAL STUDY OF CO ADSORPTION ON THREE- AND FIVE-COORDINATE AL IN OXIDE SYSTEMS
CATALYSIS LETTERS 40(3-4), 183-188 (1996)

177. ZAKHAROV, II; ZAKHAROV, VA; ZHIDOMIROV, GM.
A QUANTUM-CHEMICAL STUDY OF BETA-HYDRIDE TRANSFER REACTIONS FOR TITANIUM-CONTAINING ACTIVE SITES IN OLEFIN POLYMERIZATION
KINETICS AND CATALYSIS 37(1), 41-45 (1996)

178. ZAKHAROV, II; ZAKHAROV, VA; ZHIDOMIROV, GM.
A QUANTUM-CHEMICAL STUDY OF ACETYLENE ADDITION TO TI-H AND TI-CH3 BONDS IN HYDRIDE AND ALKYL TITANIUM COMPLEXES
KINETICS AND CATALYSIS 37(1), 35-40 (1996)

179. YEFREMENKO, IG; ZILBERBERG, IL; ZHIDOMIROV, GM; PAK, AM.
HYDROGEN ACTIVATION ON COPPER CATALYTIC SITES IN STEREOSELECTIVE ALKYNE HYDROGENATION
REACTION KINETICS AND CATALYSIS LETTERS 56(1), 77-86 (1995)

180. ZHIDOMIROV, GM; AVDEEV, VI; ZHANPEISOV, NU; ZAKHAROV, II; YUDANOV, IV.
MOLECULAR-MODELS OF ACTIVE-SITES OF C-1 AND C-2 HYDROCARBON ACTIVATION
CATALYSIS TODAY 24(3), 383-387 (1995)

181. ZHANPEISOV, NU; ZHIDOMIROV, GM; BAERNS, M.
CLUSTER QUANTUM-CHEMICAL STUDY OF THE CHEMISORPTION OF METHANE ON ZINC-OXIDE SURFACE
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL 99(1), 35-39 (1995)

182. ZHANPEISOV, NU; PAUKSHTIS, EA; ZHIDOMIROV, GM; ZAKHAROV, VA.
QUANTUM-CHEMICAL CLUSTER INVESTIGATION OF THE INTERACTION OF CARBON-MONOXIDE AND SURFACE ACID CENTERS OF HIGHLY DISPERSED MAGNESIUM-CHLORIDE

KINETICS AND CATALYSIS 36(2), 187-190 (1995)

183. MIKHEEVA, EP; RUZANKIN, SF; ZHIDOMIROV, GM.
COORDINATION BEHAVIOR OF THE CORE AND VALENCE LEVELS OF LOW-COORDINATED OXYGEN IONS ON THE SURFACE OF MAGNESIUM-OXIDE
JOURNAL OF STRUCTURAL CHEMISTRY 36(1), 13-22 (1995)

184. ZHANPEISOV, NU; ZHIDOMIROV, GM; YUDANOV, IV; KLABUNDE, KJ.
CLUSTER QUANTUM-CHEMICAL STUDY OF THE INTERACTION OF DIMETHYL METHYLPHOSPHONATE WITH MAGNESIUM-OXIDE
JOURNAL OF PHYSICAL CHEMISTRY 98(40), 10032-10035 (1994)

185. BOLSHOV, VA; VOLODIN, AM; ZHIDOMIROV, GM; SHUBIN, AA; BEDILO, AF.
RADICAL INTERMEDIATES IN THE PHOTOINDUCED FORMATION OF BENZENE CATION-RADICALS OVER H-ZSM-5 ZEOLITES
JOURNAL OF PHYSICAL CHEMISTRY 98(31), 7551-7554 (1994)

186. FILATOV, MJ; ELIZAROVA, GL; GERASIMOV, OV; ZHIDOMIROV, GM; PARMON, VN.
QUANTUM-CHEMICAL STUDY OF THE 4-ELECTRON CATALYTIC-OXIDATION OF WATER TO DIOXYGEN IN THE PRESENCE OF DINUCLEAR AND TETRANUCLEAR HYDROXIDE COMPLEXES OF COBALT(III) AND IRON(III) - INTERMEDIATES OF THE CATALYTIC CYCLE AND THEIR RELATIVE ENERGIES
JOURNAL OF MOLECULAR CATALYSIS 91(1), 71-82 (1994)

187. AVDEEV, VI; ZHIDOMIROV, GM.
THEORETICAL-ANALYSIS OF METHANE DECOMPOSITION AT THE NI(100) SURFACE
KINETICS AND CATALYSIS 35(2), 202-207 (1994)

188. ZAKHAROV, II; KOLBASINA, OI; SEMENYUK, TN; YUDANOV, IV; TYUPALO, NF; ZHIDOMIROV, GM.
AB-INITIO CALCULATIONS OF INTERACTION BETWEEN THE HYDRATED FE2+ ION AND MOLECULAR OZONE
JOURNAL OF STRUCTURAL CHEMISTRY 35(2), 176-181 (1994)

189. ZAKHAROV, II; ZAKHAROV, VA; ZHIDOMIROV, GM.
AB-INITIO CALCULATIONS FOR THE ADDITION OF ETHYLENE TO METAL HYDROGEN AND METAL METHYL BONDS IN HYDRIDE AND ALKYL COMPLEXES OF TI, AL, AND B
KINETICS AND CATALYSIS 35(1), 65-71 (1994)

190. ZHANPEISOV, NU; PAUKSHTIS, EA; ZHIDOMIROV, GM; ZAKHAROV, VA.
CLUSTER QUANTUM-CHEMICAL STUDY OF THE INTERACTION OF CARBON-MONOXIDE WITH SURFACE ACID CENTERS OF HIGHLY DISPERSED MAGNESIUM-CHLORIDE
CATALYSIS LETTERS 29(1-2), 209-215 (1994)

191. ZHANPEISOV, NU; ZHIDOMIROV, GM; BAERNS, M.
CLUSTER QUANTUM-CHEMICAL STUDY OF THE INTERACTION BETWEEN A CARBON-MONOXIDE MOLECULE AND A ZINC-OXIDE SURFACE
JOURNAL OF STRUCTURAL CHEMISTRY 35(1), 9-12 (1994)

192. MIKHEEVA, EP; RUZANKIN, SP; ZHIDOMIROV, GM.
SCF MS X-ALPHA CALCULATION FOR THE CORE-LEVEL COORDINATION BEHAVIOR OF LOW-COORDINATED OXYGEN IONS ON THE SURFACE OF MAGNESIUM-OXIDE
REACTION KINETICS AND CATALYSIS LETTERS 51(2), 357-364 (1993)

193. ZILBERBERG, IL; ZHIDOMIROV, GM; SKURATOVSKII, IY.
EFFECT OF NI(II) BINDING ON THE TAUTOMERISM OF GUANINE - A QUANTUM-CHEMICAL NDDO INVESTIGATION
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 104(1), 129-136 (1993)

194. BURGINA, EB; BALTAKHINOV, VP; BOLDYREVA, EV; STOYANOV, ES; ZHANPEISOV, NY; ZHIDOMIROV, GM.
EFFECT OF HIGH-PRESSURE ON THE VIBRATION SPECTRUM OF NITROMETHANE MOLECULES - CHANGES IN THE KINEMATICS OF THE VIBRATIONS AS A RESULT OF THE DECREASE IN THE DISTANCE BETWEEN THE MOLECULES
JOURNAL OF MOLECULAR STRUCTURE 296(1-2), 53-59 (1993)

195. FILATOV, MJ; PELMENSCHIKOV, AG; ZHIDOMIROV, GM.
ON THE NATURE OF SUPERACTIVE CENTERS IN H-ZSM-5 ZEOLITES QUANTUM-CHEMICAL CALCULATIONS (VOL 80, PG 243, 1993)
JOURNAL OF MOLECULAR CATALYSIS 81(2), 311-311 (1993)

196. ZAKHAROV, II; KOLBASINA, OI; SEMENYUK, TN; TYUPALO, NF; ZHIDOMIROV, GM.
MOLECULAR OZONE-WATER COMPLEX - AB-INITIO CALCULATION WITH INCLUSION OF ELECTRON CORRELATION
JOURNAL OF STRUCTURAL CHEMISTRY 34(3), 359-362 (1993)

197. FILATOV, MJ; PELMENSCHIKOV, AG; ZHIDOMIROV, GM.

ON THE NATURE OF SUPERACTIVE CENTERS IN H-ZSM-5 ZEOLITES - QUANTUM CHEMICAL CALCULATIONS
JOURNAL OF MOLECULAR CATALYSIS 80(2), 243-251 (1993)

198. ZAKHAROV, II; KOLBACINA, OI; SEMENYUK, TN; TYUPALO, NF; ZHIDOMIROV, GM.
ANIONIC RADICAL AND PROTONATED FORM OF MOLECULAR OZONE - A NONEMPIRICAL CALCULATION TAKING INTO ACCOUNT THE ELECTRONIC CORRELATION
JOURNAL OF STRUCTURAL CHEMISTRY 34(2), 198-202 (1993)

199. FILATOV, MJ; PELMENSCHIKOV, AG; ZHIDOMIROV, GM; HALL, WK; INUI, T; KAZANSKY, V; NOVARO, O; WICHTERLOVA, B.
ON THE NATURE OF SUPERACTIVE CENTERS IN H-FEZSM-5 ZEOLITES - QUANTUM-CHEMICAL CALCULATIONS
STUDIES IN SURFACE SCIENCE AND CATALYSIS 75, 311-319 (1993)

200. FILATOV, MJ; PELMENSCHIKOV, AG; ZHIDOMIROV, GM; HALL, WK; INUI, T; KAZANSKY, V; NOVARO, O; WICHTERLOVA, B.
ON THE NATURE OF SUPERACTIVE CENTERS IN H-FEZSM-5 ZEOLITES - QUANTUM-CHEMICAL CALCULATIONS
NEW FRONTIERS IN CATALYSIS, PTS A-C 75, 311-319 (1993)

201. FILATOV, MJ; ZILBERBERG, IL; ZHIDOMIROV, GM.
ON THE USE OF A MODEL FUNCTION OF COULOMB HOLE APPROXIMATION FOR EVALUATION OF THE COULOMB INTEGRALS IN SEMIEMPIRICAL SCF-MO METHODS
COMPUTER PHYSICS COMMUNICATIONS 73(1-3), 192-196 (1992)

202. YUDANOV, IV; ZAKHAROV, II; ZHIDOMIROV, GM.
ON THE GENERATION MECHANISM OF AROMATIC CATION-RADICALS UNDER ADSORPTION ON ZEOLITES
REACTION KINETICS AND CATALYSIS LETTERS 48(2), 411-417 (1992)

203. ZILBERBERG, IL; FILATOV, MJ; ZHIDOMIROV, GM.
COULOMB HYBRID 2-ELECTRON INTEGRALS FOR TRANSITION-METAL ATOMS - COMPARISON OF THEORETICAL INTEGRALS WITH THOSE EVALUATED FROM SPECTROSCOPIC DATA
COMPUTER PHYSICS COMMUNICATIONS 73(1-3), 205-208 (1992)

204. ZHANPEISOV, NU; PELMENSHCHIKOV, AG; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL STUDY OF THE NATURE OF HYDROXY-GROUPS ON AN MGO SURFACE
MENDELEEV COMMUNICATIONS (4), 148-149 (1992)

205. ZAKHAROV, II; AVDEEV, VI; ZHIDOMIROV, GM.
NONEMPIRICAL CLUSTER MODEL-CALCULATIONS OF THE ADSORPTION OF H2O ON NI(111)
SURFACE SCIENCE 277(3), 407-413 (1992)

206. FILATOV, MJ; ZILBERBERG, IL; ZHIDOMIROV, GM.
NDDO/MC - A NEW SEMIEMPIRICAL SCF-MO METHOD FOR TRANSITION-METAL COMPLEXES
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 44(4), 565-585 (1992)

207. ABLAEVA, MA; PELMENSHCHIKOV, AG; ZHIDOMIROV, GM; BURGINA, EB; BALTAKHINOV, VP.
NONEMPIRICAL QUANTUM-CHEMICAL CALCULATION OF THE SHIFT OF THE UPSILON(CN) FREQUENCY OF ACETONITRILE IN THE CASE OF COORDINATION WITH LEWIS ACID CENTERS
JOURNAL OF STRUCTURAL CHEMISTRY 33(5), 656-660 (1992)

208. ABLAEVA, MA; ZHIDOMIROV, GM; BURGINA, EB; BALTAKHINOV, VP; PELMENSHCHIKOV, AG; PAUKSHTIS, EA; MALYSHEVA, LV.
NONEMPIRICAL QUANTUM-CHEMICAL CALCULATIONS OF THE VIBRATIONAL-SPECTRA OF SURFACE METHOXYL GROUPS ON ALUMINUM AND SILICON-OXIDES
JOURNAL OF STRUCTURAL CHEMISTRY 33(5), 660-665 (1992)

209. AVRAMOV, PV; RUZANKIN, SP; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL SELF-CONSISTENT-FIELD-X-ALPHA SCATTERED-WAVE INVESTIGATION OF LA2CUO4 VACANT SURFACE ELECTRON-STATES
PHYSICAL REVIEW B 46(10), 6495-6500 (1992)

210. AVRAMOV, PV; RUZANKIN, SP; ZHIDOMIROV, GM.
ADSORPTION DEPENDENCE OF VACANT-ELECTRONIC-STATE DENSITIES - AS ADATOM ON A LANTHANUM OXIDE SURFACE
PHYSICAL REVIEW B 46(10), 6553-6559 (1992)

211. PLAKHUTIN, VN; SHCHEGOLEVA, LN; ZHIDOMIROV, GM.
POTENTIAL-ENERGY SURFACE FOR HIGHLY SYMMETRICAL STRUCTURES DESCRIBED IN THE HARTREE-FOCK METHOD BY NON-ROOTHAAN TYPE WAVE-FUNCTIONS
JOURNAL OF STRUCTURAL CHEMISTRY 33(5), 621-630 (1992)

212. PELMENSCHIKOV, AG; PAUKSHTIS, EA; EDISHERASHVILI, MO; ZHIDOMIROV, GM.
ON THE LOEWENSTEIN RULE AND MECHANISM OF ZEOLITE DEALUMINATION

JOURNAL OF PHYSICAL CHEMISTRY 96(17), 7051-7055 (1992)

213. ZHANPEISOV, NU; ZHIDOMIROV, GM.
MOLECULAR-STRUCTURE OF A SURFACE SUPEROXIDE RADICAL-ANION ON MGO
MENDELEEV COMMUNICATIONS (3), 111-113 (1992)

214. IRGIBAEVA, IS; BENDERSKII, VA; ZHIDOMIROV, GM; ZHANPEISOV, NU.
MINDO-3 SIMULATION OF ELECTROCHEMICAL HYDROGEN EVOLUTION - REACTION ADSORPTION OF HYDROGEN-ATOMS ON A MERCURY SURFACE
SOVIET ELECTROCHEMISTRY 28(8), 967-971 (1992)

215. ZILBERBERG, IL; FILATOV, MJ; ZHIDOMIROV, GM.
THE EVALUATION OF THE HYBRID ONE-CENTER INTEGRALS USED IN THE SEMIEMPIRICAL NDDO-TYPE METHODS FOR D-ELEMENTS FROM SPECTRA
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 42(3), 439-444 (1992)

216. ABLAEVA, MA; PELMENSHCHIKOV, AG; ZHIDOMIROV, GM; BURGINA, EB; BALTAKHINOV, VP.
ABINITIO SQM FF CALCULATIONS OF VIBRATIONAL FREQUENCIES OF ACETONITRILE COORDINATED TO LEWIS-ACIDS
REACTION KINETICS AND CATALYSIS LETTERS 47(1), 99-104 (1992)

217. ZHIDOMIROV, GM; ZHANPEISOV, NU.
ACTIVE-CENTERS OF MAGNESIUM-OXIDE SURFACE AND CALCULATIONS OF DISSOCIATIVE CHEMISORPTION OF METHANE ON MODIFIED MGO
CATALYSIS TODAY 13(4), 517-522 (1992)

218. AVDEEV, VI; ZAKHAROV, II; ZHIDOMIROV, GM; NESHEV, NM; PROINOV, EI.
ELECTRONIC-STRUCTURE OF OH ADSORBED ON NICKEL
JOURNAL OF STRUCTURAL CHEMISTRY 33(2), 179-185 (1992)

219. AVDEEV, VI; ZAKHAROV, II; ZHIDOMIROV, GM.
THEORETICAL-ANALYSIS OF DISSOCIATIVE ADSORPTION OF H2O ON NI(100)
JOURNAL OF STRUCTURAL CHEMISTRY 33(2), 185-190 (1992)

220. PLAKHUTIN, BN; ZHIDOMIROV, GM; ARBUZNIKOV, AV.
VECTOR COUPLING-COEFFICIENTS FOR CALCULATIONS OF TRANSITION-METAL ATOMS AND IONS BY THE SCF COUPLING OPERATOR METHOD
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 41(2), 311-325 (1992)

221. ZHIDOMIROV, GM; ZHANPEISOV, NU.
QUANTUM-CHEMICAL STUDY OF COMPLEXES WITH HYDROGEN-BONDS
KHIMICHESKAYA FIZIKA 11(5), 670-677 (1992)

222. ZHANPEISOV, NU; ZHIDOMIROV, GM.
PARAMETRIZATION OF THE SEMIEMPIRICAL MINDO/3 QUANTUM-CHEMICAL METHOD FOR ZINC-CONTAINING COMPOUNDS
JOURNAL OF STRUCTURAL CHEMISTRY 33(1), 128-130 (1992)

223. ZHANPEISOV, NU; ZHIDOMIROV, GM.
CLUSTER QUANTUM CHEMICAL STUDY OF DIHYDROGEN, METHANE AND WATER-MOLECULES - INTERACTIONS WITH PURE AND LITHIUM DOPED MAGNESIUM-OXIDE
PHYSICS AND CHEMISTRY OF FINITE SYSTEMS : FROM CLUSTERS TO CRYSTALS, VOLS 1 AND 2 374, 1177-1182 (1992)

224. ZAKHAROV, II; ZHIDOMIROV, GM; ZAKHAROV, VA.
NONEMPIRICAL CALCULATIONS FOR THE INTERACTION OF DIHYDROGEN WITH HYDRIDE AND ALKYL COMPLEXES OF BORON, ALUMINUM AND TITANIUM
JOURNAL OF MOLECULAR CATALYSIS 68(2), 149-157 (1991)

225. AVDEEV, VI; ZAKHAROV, II; ZHIDOMIROV, GM; NESHEV, NM; PROINOV, EI.
ABINITIO CALCULATIONS FOR ADSORBED STATE OF OH GROUP ON NI(110)
REACTION KINETICS AND CATALYSIS LETTERS 45(1), 61-66 (1991)

226. PLAKHUTIN, BN; SHCHEGOLEVA, LN; ZHIDOMIROV, GM.
INADEQUACY OF ONE-ELECTRON APPROACH FOR INVESTIGATING ANTIAROMATIC MOLECULES AND THEIR ISOMERIZATION-REACTIONS
JOURNAL OF STRUCTURAL CHEMISTRY 32(5), 641-651 (1991)

227. ZHANPEISOV, NU; PELMENSHCHIKOV, AG; ZHIDOMIROV, GM.
CLUSTER QUANTUM CHEMICAL STUDY OF THE REACTION OF MOLECULES WITH A MAGNESIUM-OXIDE SURFACE .2. MOLECULAR AND DISSOCIATIVE ADSORPTION OF H2O
KINETICS AND CATALYSIS 32(4), 875-877 (1991)

228. ZHDANOV, VP; GRITSENKO, OV; ZHIDOMIROV, GM.
VACUUM TUNNELING CURRENT FROM A LARGE ADSORBED MOLECULE
PHYSICS LETTERS A 153(1), 40-42 (1991)
229. BOLSHOV, VA; VOLODIN, AM; MARYASOV, AG; YUDANOV, VF; ZHIDOMIROV, GM.
INSITU ESR MEASUREMENTS OF THE FORMATION OF FREE-RADICALS UNDER HIGH-TEMPERATURE ADSORPTION OF BENZENE ON H-ZSM-5 ZEOLITES
DOKLADY AKADEMII NAUK SSSR 316(1), 141-144 (1991)
230. ZAKHAROV, II; ZHIDOMIROV, GM.
LEWIS ACID SITES IN DIVALENT SILICON - QUANTUM CHEMICAL STUDY OF THE REACTION WITH CO
KINETICS AND CATALYSIS 32(1), 27-31 (1991)
231. FILATOV, MJ; TALSI, EP; GRITSENKO, OV; ZHIDOMIROV, GM; ZAMARAEV, KI.
PALLADIUM SUPEROXIDO COMPLEXES - IN WHAT WAY (SIGMA-OR-PI) IS O-2(-) COORDINATED - A QUANTUM CHEMICAL APPROACH
JOURNAL OF THE CHEMICAL SOCIETY-DALTON TRANSACTIONS (11), 3265-3269 (1990)
232. MEDIN, AS; BOROVKOV, VY; KAZANSKY, VB; PELMENTSCHIKOV, AG; ZHIDOMIROV, GM.
ON THE UNUSUAL MECHANISM OF LEWIS ACIDITY MANIFESTATION IN HZSM-5 ZEOLITES
ZEOLITES 10(7), 668-673 (1990)
233. MALKINA, OL; GRITSENKO, OV; ZHIDOMIROV, GM.
A NEW APPROXIMATION FOR SLATER AVERAGED HARTREE-FOCK EXCHANGE POTENTIAL
CHEMICAL PHYSICS LETTERS 171(3), 191-196 (1990)
234. ZHANPEISOV, NU; PELMENSHCHIKOV, AG; ZHIDOMIROV, GM.
CLUSTER QUANTUM CHEMICAL STUDY OF INTERACTION OF MOLECULES WITH A MAGNESIUM-OXIDE SURFACE .1. DISSOCIATIVE CHEMISORPTION OF HYDROGEN AND METHANE MOLECULES
KINETICS AND CATALYSIS 31(3), 491-496 (1990)
235. ZAKHAROV, II; ZHIDOMIROV, GM.
LEWIS ACID SITES OF BIVALENT SILICON AND QUANTUM-CHEMICAL STUDIES OF INTERACTION WITH CO
REACTION KINETICS AND CATALYSIS LETTERS 41(1), 59-64 (1990)
236. MALKIN, VG; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL CALCULATIONS OF SI-29 CHEMICAL-SHIFTS IN ZEOLITES
ZEOLITES 10(3), 207-209 (1990)
237. MALKIN, VG; CHESNOKOV, VV; PAUKSHTIS, EA; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL CALCULATIONS OF C-13 CHEMICAL-SHIFTS OF THE ALKOXIDE FORM IN ZEOLITES
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 112(2), 666-669 (1990)
238. KLIMKO, GT; MESTECHKIN, MM; PLAKHUTIN, BN; ZHIDOMIROV, GM; EVARESTOV, RA.
THE ORIGIN OF ENERGY FUNCTIONAL IN ROOTHAAN OPEN-SHELL SCF THEORY
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 37(1), 35-50 (1990)
239. GORB, LG; ILCHENKO, NN; GREBENYUK, AG; GONCHARUK, VV; ZHIDOMIROV, GM.
ON CHEMICAL NATURE OF THE LEWIS ACID CENTER OF DEHYDROXYLATED ALUMOSILICATE CATALYSTS
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 26(3), 383-383 (1990)
240. PELMENSHCHIKOV, AG; EDISHERASHVILI, MO; ZHIDOMIROV, GM; KHUROSHVILI, DV; TSITSISHVILI, GN.
QUANTUM-CHEMICAL STUDIES OF STRUCTURAL STATES OF ALO3 FRAGMENTS IN OXIDE LATTICES
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 26(3), 334-340 (1990)
241. ZHANPEISOV, N. U.; PELMENCHIKOV, A. G.; ZHIDOMIROV, G. M..
CLUSTER QUANTUM CHEMICAL STUDY OF THE INTERACTION OF MOLECULES WITH MGO SURFACE. I. DISSOCIATIVE CHEMISORPTIONS OF H2AND CH4
KINET. KATAL. 31, 563 (1990)
242. ZOLOTOVSKII, BP; PARAMZIN, SM; PELMENSHCHIKOV, AG; PAUKSHTIS, EA; KLEVTSOV, DP; ERMOLAEVA, NV; BUYANOV, RA; ZHIDOMIROV, GM.
RELATIONSHIPS IN FORMATION OF PAIRED LEWIS CENTERS IN ALUMINUM-OXIDE, AND THEIR ADSORPTION PROPERTIES
KINETICS AND CATALYSIS 30(6), 1252-1256 (1989)
243. FILATOV, MJ; GRITSENKO, OV; ZHIDOMIROV, GM.
CNDO-S2 - A NEW SEMIEMPIRICAL SCF-MO METHOD FOR TRANSITION-METAL ORGANOMETALLICS
JOURNAL OF MOLECULAR CATALYSIS 54(3), 462-477 (1989)
244. PELMENSHCHIKOV, AG; PAUKSHTIS, EA; STEPANOV, VG; PAVLOV, VI; YURCHENKO, EN; IONE, KG; ZHIDOMIROV, GM; BERAN, S.
EFFECT OF STRUCTURAL AND CHEMICAL FACTORS ON THE ACIDITY AND IR SPECTROSCOPIC CHARACTERISTICS

OF BRIDGING OH GROUPS IN ZEOLITES
JOURNAL OF PHYSICAL CHEMISTRY 93(18), 6725-6730 (1989)

245. SHUBIN, AA; ZHIDOMIROV, GM.
CALCULATION OF ANISOTROPICALLY BROADENED EPR-SPECTRA - SHAPE OF THE EPR-SPECTRUM OF A NITROXIDE RADICAL IN THE 2-MILLIMETER RANGE
JOURNAL OF STRUCTURAL CHEMISTRY 30(3), 414-417 (1989)

246. KONDRATENKO, AV; FOMIN, ES; NEMANOVA, VI; RUZANKIN, SF; ZHIDOMIROV, GM; MAZALOV, LN.
CONTINUUM STATES, XANES, AND EXAFS FOR VO43-, CRO42-, AND MNO4-
JOURNAL OF STRUCTURAL CHEMISTRY 30(2), 249-252 (1989)

247. KONKOV, KA; ZHIDOMIROV, GM; KALIYA, OL; KHLESKOV, VI; IVANOV, YV.
QUANTUM-CHEMICAL ANALYSIS OF ACID-BASE PROPERTIES OF METAL-COMPLEXES OF AZAPORPHYRINS BY THE INDO METHOD
JOURNAL OF STRUCTURAL CHEMISTRY 30(2), 189-194 (1989)

248. ZELENKOVSKII, VM; MARDILOVICH, PP; ZHIDOMIROV, GM.
NON-EMPIRICAL CALCULATIONS OF ADSORBABILITY OF PAIRED LEWIS ACID SITES OF ALUMINA
REACTION KINETICS AND CATALYSIS LETTERS 38(1), 73-77 (1989)

249. ZHANPEISOV, NU; ZHIDOMIROV, GM.
APPLICATION OF MINDO-3-HB METHOD TO EVALUATION OF ACTIVATION-ENERGY OF INTRAMOLECULAR PROTON-TRANSFER IN MALONALDEHYDE
REACTION KINETICS AND CATALYSIS LETTERS 38(2), 395-397 (1989)

250. KONKOV, KA; ZHIDOMIROV, GM; KHLESKOV, VI; KOPRANENKOV, VN; IVANOV, YV.
QUANTUM-CHEMICAL ANALYSIS OF SPECTRA FOR METAL ASAPORPHYRIN COMPLEXES BY THE INDO/S METHOD
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 25(4), 471-476 (1989)

251. ILCHENKO, NN; GREBENYUK, AG; GORB, LG; GONCHARUK, VV; ZHIDOMIROV, GM.
CLUSTER QUANTUM-CHEMICAL MODELS OF HYPERVALENT COORDINATION ENVIRONMENT OF ATOMS IN THE STRUCTURE OF ALUMINUM-OXIDES
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 25(5), 581-586 (1989)

252. OSIPOVA, GE; YURCHENKO, EN; BALTAKHINOV, VP; PAVLOV, VI; ZHIDOMIROV, GM.
FORCE-FIELD CALCULATIONS FOR S, SE, AND TE HEXAFLUORIDES
JOURNAL OF STRUCTURAL CHEMISTRY 30(1), 40-43 (1989)

253. GRITSENKO, OV; DANILOVA, SV; ZHANPEISOV, NU; MALKIN, VG; ZHIDOMIROV, GM.
A COMBINED METHOD OF SCF-MO LCAO AND CORRELATION DENSITY FUNCTIONAL AS APPLIED TO ADSORPTION OF ATOMIC-HYDROGEN BY LITHIUM CLUSTERS
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 25(4), 385-392 (1989)

254. KON'KOV, K.A.; ZHIDOMIROV, G.M.; KHLESKOV, V.I.; KOPRANENKOV, V.N.; IVANOV, YU.V..
QUANTUM-CHEMICAL ANALYSIS OF THE SPECTRA OF METAL COMPLEXES OF AZAPORPHYRINS BY THE INDO/S METHOD
THEORETICAL AND EXPERIMENTAL CHEMISTRY 25(4), 436 (1989)

255. PELMENSHCHIKOV, AG; ZHIDOMIROV, GM; ZAMARAEV, KI.
QUANTUM-CHEMICAL INTERPRETATION OF INTRAZEOLITE CHEMISTRY PHENOMENA
ZEOLITES : FACTS, FIGURES, FUTURE, PTS A & B 49, 741-752 (1989)

256. MALKIN, VG; GRITSENKO, OV; ZHIDOMIROV, GM.
SI-29 NMR - A NEW APPROACH TO THE ANALYSIS OF CHEMICAL-SHIFT VARIATIONS
CHEMICAL PHYSICS LETTERS 152(1), 44-49 (1988)

257. KONDRATENKO, AV; NEIMAN, KM; GUTSEV, GL; ZHIDOMIROV, GM; RUZANKIN, SF.
QUANTUM-CHEMISTRY AND SPECTROSCOPY OF HIGHLY EXCITED-STATES OF COORDINATION-COMPOUNDS
JOURNAL OF STRUCTURAL CHEMISTRY 29(6), 899-910 (1988)

258. MALKIN, VG; ZHIDOMIROV, GM.
SCF X-ALPHA DW NUCLEAR MAGNETIC SCREENING TENSOR CALCULATIONS
JOURNAL OF STRUCTURAL CHEMISTRY 29(5), 684-687 (1988)

259. PLAKHUTIN, BN; ZHIDOMIROV, GM.
CHARACTER OF APPROXIMATIONS IN THE BASIS OF THE HALF-ELECTRON METHOD
ZHURNAL FIZICHESKOI KHIMII 62(7), 1724-1740 (1988)

260. AVDEEV, VI; ZHIDOMIROV, GM.
THEORETICAL-ANALYSIS OF THE 1ST STEP IN THE HYDROGENATION OF CARBON ON AN NI(100) SURFACE
KINETICS AND CATALYSIS 29(4), 692-698 (1988)

261. FILATOV, MY; GRITSENKO, OV; ZHIDOMIROV, GM.

NEW SEMIEMPIRICAL SCF-MO METHOD FOR CALCULATING ORGANOMETALLIC COMPOUNDS
JOURNAL OF STRUCTURAL CHEMISTRY 29(3), 349-356 (1988)

262. TSINTSADZE, GV; ZHIDOMIROV, GM; MELADZE, MA; PELMENSHCHIKOV, AG; KVEZERELI, EA; ZHANPEISOV, NU; NARIMANIDZE, AP.
QUANTUM CHEMICAL STUDY OF THE PROTON ACCEPTOR PROPERTIES OF AMIDES AND HYDRAZIDES OF NICOTINIC AND ISONICOTINIC ACIDS
BULLETIN OF THE ACADEMY OF SCIENCES OF THE USSR DIVISION OF CHEMICAL SCIENCE 37(4), 810-812 (1988)

263. NEMANOVA, VI; KONDRATENKO, AV; RUZANKIN, SF; BAUSK, NV; ZHIDOMIROV, GM; MAZALOV, LN.
XANES FOR PD AND PT IN SQUARE AND OCTAHEDRAL CHLORIDE COMPLEXES
JOURNAL OF STRUCTURAL CHEMISTRY 29(2), 221-228 (1988)

264. MARDILOVICH, PP; ZELENKOVSKII, VM; LYSENKO, GN; TROKHIMETZ, AI; ZHIDOMIROV, GM.
ON THE NATURE OF SURFACE SITES FOR HETEROLYTIC DISSOCIATION OF HYDROGEN ON AL2O3
REACTION KINETICS AND CATALYSIS LETTERS 36(1), 107-112 (1988)

265. PLAKHUTIN, BN; ZHIDOMIROV, GM.
THEORETICAL-ANALYSIS OF MAGNETIC AND ELECTRICAL SUPERFINE INTERACTIONS ON NUCLEI OF COPPER(II) H-1, H-2 BIS-ACETYLACETONATE
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 24(2), 149-155 (1988)

266. ZELENKOVSKII, VM; MARDILOVICH, PP; LYSENKO, GN; TROKHIMETS, AI; ZHIDOMIROV, GM.
ADSORPTIVITY OF LEWIS ACIDIC CENTERS OF AL2O3 BASED ON ABINITIO CALCULATIONS
ZHURNAL FIZICHESKOI KHIMII 61(12), 3369-3371 (1987)

267. PLAKHUTIN, BN; ZHIDOMIROV, GM; MESTECHKIN, MM.
CONSTRUCTION AND PROPERTIES OF SUPPLEMENTARY SOLUTIONS OF THE HARTREE-FOCK EQUATIONS FOR THE CLOSED SHELL
JOURNAL OF STRUCTURAL CHEMISTRY 28(6), 813-820 (1987)

268. FILATOV, MJ; GRITSENKO, OV; ZHIDOMIROV, GM.
CNDO-S2 - A SEMIEMPIRICAL SCF-MO METHOD FOR TRANSITION-METAL ORGANOMETALLICS
THEORETICA CHIMICA ACTA 72(3), 211-222 (1987)

269. KONDRATENKO, AV; NEMANOVA, VI; RUZANKIN, SF; BAUSK, NV; ZHIDOMIROV, GM; MAZALOV, LN.
SCF X-ALPHA-SW CALCULATIONS OF XANES AND EXAFS OF PT ATOM IN CHLORIDE COMPLEXES
JOURNAL OF STRUCTURAL CHEMISTRY 28(5), 645-648 (1987)

270. GRITSENKO, OV; ZHIDOMIROV, GM.
CORRELATION-ENERGY CORRECTION AS A DENSITY FUNCTIONAL - A MODEL OF THE PAIR DISTRIBUTION FUNCTION AND ITS APPLICATION TO THE 1ST-ROW AND 2ND-ROW ATOMS AND HYDRIDES
CHEMICAL PHYSICS 116(1), 21-32 (1987)

271. NEMANOVA, VI; KONDRATENKO, AV; RUZANKIN, SF; BAUSK, NV; ZHIDOMIROV, GM; MAZALOV, LN.
XANES OF THE PD AND PT ATOMS IN SQUARE AND OCTAHEDRAL CHLORIDE COMPLEXES
CHEMICAL PHYSICS 116(1), 61-68 (1987)

272. ZAMARAEV, KI; ZHIDOMIROV, GM.
ACTIVE-SITES AND THE ROLE OF THE MEDIUM IN HOMOGENEOUS, HETEROGENEOUS AND ENZYMATIC CATALYSIS
IZVESTIYA SIBIRSKOGO OTDELENIYA AKADEMII NAUK SSSR SERIYA KHIMICHESKIKH NAUK (4), 3-17 (1987)

273. KONKOV, KA; ZHIDOMIROV, GM; IVANOV, YV.
SEMIEMPIRICAL QUANTUM-CHEMICAL STRUCTURE AND ELECTRONIC-SPECTRUM CALCULATIONS FOR TRANSITION-METAL COMPLEXES
JOURNAL OF STRUCTURAL CHEMISTRY 28(4), 596-597 (1987)

274. PELMENSHCHIKOV, AG; PAVLOV, VI; ZHIDOMIROV, GM; BERAN, S.
EFFECTS OF STRUCTURAL AND CHEMICAL CHARACTERISTICS OF ZEOLITES ON THE PROPERTIES OF THEIR BRIDGING HYDROXYL-GROUPS
JOURNAL OF PHYSICAL CHEMISTRY 91(12), 3325-3327 (1987)

275. GRITSENKO, OV; DANILOVA, SV; ZHANPEISOV, NU; MALKIN, VG; ZHIDOMIROV, GM.
ON THE EVALUATION OF THE CORRELATION-ENERGY AND THE TOTAL NONRELATIVISTIC BORN-OPPENHEIMER ENERGY FOR THE WATER MOLECULE
CHEMICAL PHYSICS LETTERS 134(5), 423-427 (1987)

276. GRITSENKO, OV; ZHIDOMIROV, GM.
EXCHANGE-CORRELATION DENSITY-FUNCTIONS IN THE THEORY OF MANY-ELECTRON SYSTEMS
JOURNAL OF STRUCTURAL CHEMISTRY 28(2), 279-307 (1987)

277. PELMENSHCHIKOV, AG; ZHIDOMIROV, GM; BERAN, S; TINO, J.

MOLECULAR APPROACH IN THE STUDY OF THE PROCESSES OF FORMATION OF THE LATTICE OF OXIDES - CHARACTERISTIC FEATURES OF COORDINATION OF ALO3 STRUCTURAL ELEMENTS
PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE 99(1), 57-64 (1987)

278. GRITSENKO, OV; ZHIDOMIROV, GM.
ON THE DETERMINATION OF THE 1ST-ORDER DENSITY-MATRIX FROM THE DIFFRACTION EXPERIMENT DATA
DOKLADY AKADEMII NAUK SSSR 293(5), 1162-1166 (1987)

279. PELMENSHCHIKOV, AG; PAUKSHTIS, EA; ZHANPEISOV, NU; PAVLOV, VI; ZHIDOMIROV, GM.
COMPARATIVE DISCUSSION OF NH4+ FORMATION MECHANISMS ON OXIDE SURFACES AND IN ACIDIC MEDIA
REACTION KINETICS AND CATALYSIS LETTERS 33(2), 423-428 (1987)

280. PLAKHUTIN, BN; KLIMKO, GT; MESTECHKIN, MM; ZHIDOMIROV, GM.
ON RELATION OF THE ENERGY FUNCTIONAL FOR OPEN-SHELL IN THE ROOTHAAN METHOD TO THE SYSTEM SYMMETRY
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 23(2), 129-134 (1987)

281. ZELENKOVSKII, VM; MARDILOVICH, PP; LYSENKO, GN; TROKHIMETS, AI; ZHIDOMIROV, GM.
NON-EMPIRICAL CALCULATIONS FOR THE PROBABLE COORDINATIVE BINDING OF ELECTRON-DONOR MOLECULES BY (ALO4) TETRAHEDRA
REACTION KINETICS AND CATALYSIS LETTERS 34(2), 277-281 (1987)

282. ZHANPEISOV, NU; PELMENSHCHIKOV, AG; PAUKSHTIS, EA; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL STUDY OF THE MECHANISM OF FORMATION OF THE PYRIDINIUM ION ON AN ALUMINOSILICATE SURFACE AND IN THE LIQUID-PHASE
KINETICS AND CATALYSIS 28(1), 173-176 (1987)

283. ZHIDOMIROV, GM; PELMENSHCHIKOV, AG; ZHANPEISOV, NU; GREBENYUK, AG.
CLUSTER APPROACH TO QUANTUM-CHEMICAL CALCULATIONS OF CHEMISORPTION AND HETEROGENEOUS CATALYTIC-SYSTEMS
KINETICS AND CATALYSIS 28(1), 74-86 (1987)

284. ZHANPEISOV, NU; PELMENSHCHIKOV, AG; ZHIDOMIROV, GM.
A FORM OF THE MINDO/3 METHOD FOR HYDROGEN-BONDED COMPLEXES
JOURNAL OF STRUCTURAL CHEMISTRY 28(1), 1-5 (1987)

285. PALMENSHCHIKOV, AG; ZHANPEISOV, NU; PAUKSHTIS, EA; MALYSHEVA, LV; ZHIDOMIROV, GM; ZAMARAEV, KI.
ON THE NATURE OF TRANSITION-STATE IN THE REACTIONS OF PROTON-ACID HETEROGENEOUS ORGANIC CATALYSIS
DOKLADY AKADEMII NAUK SSSR 293(4), 910-920 (1987)

286. PLAKHUTIN, B.N.; KLIMKO, G.T.; MESTECHKIN, M.M.; ZHIDOMIROV, G.M..
THE RELATION BETWEEN THE OPEN SHELL ENERGY FUNCTIONAL IN THE ROOTHAAN METHOD AND THE SYMMETRY OF THE SYSTEM
THEORETICAL AND EXPERIMENTAL CHEMISTRY 23(2), 123 (1987)

287. GRITSENKO, OV; BAGATURYANTS, AA; ZHIDOMIROV, GM.
ON THE CONSTRUCTION OF THE EFFECTIVE PAIR CORRELATION-FUNCTION WITH THE FIXED ZERO VALUE AT THE POINTS WHERE 2 ELECTRON POSITIONS COINCIDE
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 30(6), 791-797 (1986)

288. GRITSENKO, OV; ZHIDOMIROV, GM.
A NEW CORRELATION-ENERGY INTERPOLATION FUNCTIONAL FOR MANY-ELECTRON SYSTEMS IN THE HOMOGENEOUS ELECTRON-GAS MODEL - THE RATIO OF PARAMAGNETIC AND FERROMAGNETIC STATE ENERGIES VERSUS GAS-DENSITY
PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS 138(1), 161-169 (1986)

289. ZHIDOMIROV, GM; PELMENSHCHIKOV, AG.
MOLECULAR-MODELS IN THE QUANTUM-CHEMICAL INVESTIGATION OF THE STRUCTURE OF DEFECT CENTERS ON OXIDE CATALYSTS
JOURNAL OF STRUCTURAL CHEMISTRY 27(6), 971-978 (1986)

290. PAUKSHTIS, EA; PANKRATEV, YD; PELMENSHCHIKOV, AG; BURGINA, EB; TURKOV, VM; YURCHENKO, EN; ZHIDOMIROV, GM.
PECULIARITIES OF THE PROTONATION OF NITROGEN BASES ON THE SURFACE OF ZEOLITES
KINETICS AND CATALYSIS 27(6), 1249-1253 (1986)

291. ZAKHAROV, II; ZHIDOMIROV, GM.
CORRELATION-ENERGY IN BONDS - DEVELOPMENT OF A SEMIEMPIRICAL SCHEME - THE CNDO-CMP METHOD
JOURNAL OF STRUCTURAL CHEMISTRY 27(4), 503-509 (1986)

292. PLAKHUTIN, BN; ZHIDOMIROV, GM.

CONSTRUCTING FUNCTIONS WITH THE CORRECT SYMMETRY FOR TERMS OF NON-ROOTHAAN TYPE IN THE RESTRICTED HARTREE-FOCK METHOD
JOURNAL OF STRUCTURAL CHEMISTRY 27(2), 179-183 (1986)

293. ZHIDOMIROV, GM; KAZANSKY, VB.
QUANTUM-CHEMICAL CLUSTER-MODELS OF ACID-BASE SITES OF OXIDE CATALYSTS
ADVANCES IN CATALYSIS 34, 131-202 (1986)

294. PELMENSHCHIKOV, AG; ZHIDOMIROV, GM.
QUALITATIVE QUANTUM-CHEMICAL MODELS FOR SURFACE OH GROUPS OF OXIDES
REACTION KINETICS AND CATALYSIS LETTERS 31(1), 85-91 (1986)

295. SENCHENYA, IN; PELMENSHCHIKOV, AG; ZHIDOMIROV, GM; KAZANSKII, VB.
MINDO/3 STUDIES OF SURFACE OH GROUPS OF ALUMINA
REACTION KINETICS AND CATALYSIS LETTERS 31(1), 101-105 (1986)

296. ZAKHAROV, II; ZHIDOMIROV, GM.
CALCULATION OF ATOMIC ADSORPTION OF CARBON ON NI(100) BY SEMIEMPIRICAL SCF METHOD ACCOUNTING FOR THE CORRELATION OF MOLECULAR PAIRS
REACTION KINETICS AND CATALYSIS LETTERS 31(2), 303-307 (1986)

297. ZHIDOMIROV, GM; CHUVYLKIN, ND.
QUANTUMCHEMICAL METHODS IN CATALYSIS
RUSS CHEM REV 55(3), 153 (1986)

298. TSINTSADZE, GV; ZHIDOMIROV, GM; KVEZERELI, EA; PELMENSHCHIKOV, AG; ZHANPIISOV, NU; MELADZE, MA.
QUANTUM-CHEMICAL STUDY OF THE PROPERTIES OF THE PEPTIDE-BOND IN PROTONATED FORMAMIDE
BULLETIN OF THE ACADEMY OF SCIENCES OF THE USSR DIVISION OF CHEMICAL SCIENCE 34(11), 2425-2427 (1985)

299. PELMENCHIKOV, AG; PAVLOV, VI; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL COMPARISON OF THE COORDINATION ABILITIES OF B AND AL IN OXIDES WITHIN THE FRAMEWORK OF THE MOLECULAR-MODEL
PHYSICA STATUS SOLIDI B-BASIC RESEARCH 130(1), K1-K4 (1985)

300. PUSHKARCHUK, AL; MARDILOVICH, PP; TROKHIMETS, AI; GAGARIN, SG; ZHIDOMIROV, GM.
BAND-STRUCTURE VARIATION OF THE (0001) FACE FOR CORUNDUM DURING FORMATION AND HYDRATION
PHYSICA STATUS SOLIDI B-BASIC RESEARCH 129(2), K181-K185 (1985)

301. MIKHALKO, VK; ZHIDOMIROV, GM; LEBEDEV, OL.
INFLUENCE OF OXYGEN ON THE ELECTRONIC-SPECTRA OF ORGANIC-COMPOUNDS .2. CALCULATIONS OF THE SPECTRUM OF THE BENZENE OXYGEN MOLECULAR-COMPLEX
JOURNAL OF STRUCTURAL CHEMISTRY 25(1), 1-5 (1984)

302. PUSHKARCHUK, AL; MARDILOVICH, PP; TROKHIMETS, AI; ZHIDOMIROV, GM; GAGARIN, SG.
THE ENERGY-BAND STRUCTURE OF THE CORUNDUM (0001) SURFACE WITH DIFFERENT EXTENT OF HYDROXYLATION
PHYSICA STATUS SOLIDI B-BASIC RESEARCH 124(2), 699-705 (1984)

303. ZELENKOVSKII, VM; ZHIDOMIROV, GM; KAZANSKII, VB.
NONEMPIRICAL CALCULATIONS OF WATER-ADSORPTION ON BRIDGED STRUCTURAL FRAGMENTS OF ALUMINOSILICATE
REACTION KINETICS AND CATALYSIS LETTERS 24(1-2), 15-17 (1984)

304. MASTIKHIN, VM; MUDRAKOVSKII, IL; PELMENTSCHIKOV, AG; ZHIDOMIROV, GM.
NMR-STUDY OF PROPYLENE ADSORPTION ON GAMMA-AL2O3
SURFACE SCIENCE 144(2-3), 550-558 (1984)

305. GORB, LG; ABRONIN, IA; KHARCHEVNIKOVA, NV; ZHIDOMIROV, GM.
MUTUAL CORRESPONDENCE OF DIFFERENT METHODS OF CONTROL OF ELECTROSTATICAL INPUT INTO THE SOLVATION ENERGY IN QUANTUMCHEMICAL CALCULATIONS
ZHURNAL FIZICHESKOI KHIMII 58(1), 9-19 (1984)

306. ZELENKOVSKII, VM; ZHIDOMIROV, GM; KAZANSKII, VB.
QUANTUM-CHEMICAL STUDY OF THE ADSORPTION OF MOLECULAR-HYDROGEN ON A LEWIS ACIDIC CENTER
ZHURNAL FIZICHESKOI KHIMII 58(7), 1788-1790 (1984)

307. MIKHALKO, VK; ZHIDOMIROV, GM; LEBEDEV, OL.
OXYGEN INFLUENCE ON ELECTRONIC SPECTRUMS OF ORGANIC-COMBINATIONS
ZHURNAL FIZICHESKOI KHIMII 58(8), 1857-1867 (1984)

308. GAGARIN, SG; ZHIDOMIROV, GM.
PRINCIPLE OF OPTIMUM OF MOLECULE ELECTRON MODIFICATION DURING COORDINATION

ZHURNAL FIZICHESKOI KHIMII 58(12), 3010-3014 (1984)

309. GORB, LG; ABRONIN, IA; KORSUNOV, VA; ZHIDOMIROV, GM; LITVINOV, VP.
ROLE OF CHARGE-TRANSFER IN AROMATIC ELECTROPHILIC SUBSTITUTION-REACTIONS
BULLETIN OF THE ACADEMY OF SCIENCES OF THE USSR DIVISION OF CHEMICAL SCIENCE 33(5), 991-996 (1984)

310. ZELENKOVSKII, VM; ZHIDOMIROV, GM; KAZANSKII, VB.
NON-EMPIRICAL CALCULATION O COORDINATE BONDS OF MOLECULES OF WATER AND AMMONIA BY SILICON ATOMS OF SILANOL GROUPS
ZHURNAL FIZICHESKOI KHIMII 58(8), 1945-1948 (1984)

311. TSITSISHVILI, GV; KHUROSHVILI, DV; ZHIDOMIROV, GM; PELMENSCHIKOV, AG.
QUANTUM-CHEMICAL EXAMINATION OF THE FACTORS RULE IN TERMS OF SIMPLEST CLUSTER CALCULATION APPROACHES
REACTION KINETICS AND CATALYSIS LETTERS 25(1-2), 83-86 (1984)

312. PELMENSHCHIKOV, AG; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL STUDIES OF ACIDIC CENTERS IN ALUMINOPHOSPHATES
REACTION KINETICS AND CATALYSIS LETTERS 23(3-4), 295-299 (1983)

313. ANIKIN, NA; BAGATURYANTS, AA; ZHIDOMIROV, GM; KAZANSKII, VB.
NON-EMPIRICAL QUANTUM STUDY OF THE MODEL REACTION OF CO INTRODUCTION INTO THE PD-H BOND
ZHURNAL FIZICHESKOI KHIMII 57(3), 653-656 (1983)

314. LEBEDEV, VL; BAGATURYANTS, AA; ZHIDOMIROV, GM; KAZANSKII, VB.
QUANTUM-CHEMICAL STUDY OF CH4 ACTIVATION BY PT(II) COMPLEXES
ZHURNAL FIZICHESKOI KHIMII 57(5), 1057-1067 (1983)

315. PELMENSHCHIKOV, AG; SENCHENYA, II; ZHIDOMIROV, GM.
DEPENDENCE OF CALCULATED PHYSICOCHEMICAL CHARACTERISTICS OF A MODEL SURFACE CLUSTER AND ITS INTERACTION WITH THE SIMPLEST MOLECULES ON THE METHOD OF ACCOUNTING FOR THE BOUNDARY-CONDITIONS AND ON THE CLUSTER SIZE
KINETICS AND CATALYSIS 24(4), 699-703 (1983)

316. KORSUNOV, VA; CHUVYLKIN, ND; ZHIDOMIROV, GM; KAZANSKII, VB.
CLUSTER QUANTUM-MECHANICAL ANALYSIS OF SPECTROSCOPIC AND ACTIVATION PARAMETERS OF SURFACE COMPLEXES ON OXIDES .2. MECHANISM OF PHOTOLUMINESCENCE OF SURFACE FORMS OF VO43-
KINETICS AND CATALYSIS 24(3), 483-487 (1983)

317. PLAKHUTIN, BI; ZHIDOMIROV, GM; ZAMARAEV, KI.
INDO CALCULATIONS OF SPIN-HAMILTONIAN CONSTANTS IN TRANSITION-METAL COMPLEXES - INFLUENCE OF STRUCTURAL DISTORTIONS AND ADDUCT FORMATION ON G-TENSOR OF COPPER(II) BIS-ACETYLACETONATE
JOURNAL OF STRUCTURAL CHEMISTRY 24(2), 169-176 (1983)

318. PELMENSHCHIKOV, AG; SENCHENYA, IN; ZHIDOMIROV, GM; KAZANSKII, VB.
QUANTUM CHEMICAL INVESTIGATION OF LEWIS ACID SITES OF ALUMINOSILICATES
KINETICS AND CATALYSIS 24(1), 196-198 (1983)

319. SENCHENYA, IN; MIKHEIKIN, ID; ZHIDOMIROV, GM; TROKHIMETS, AI.
CLUSTER-MODEL CALCULATIONS FOR CHEMISORPTION AND THE INDIVIDUAL STEPS OF CATALYTIC REACTIONS .14. LEWIS ACID SITES
KINETICS AND CATALYSIS 24(1), 27-32 (1983)

320. STEPANYUK, VS; ZHIDOMIROV, GM; KATSNELSON, AA; SHPOTIN, IS; YASTREBOV, LI.
CLUSTERS IN ALLOYED CATALYSTS ON THE BASIS OF COPPER
ZHURNAL FIZICHESKOI KHIMII 57(5), 1193-1197 (1983)

321. SHPOTIN, IS; ZHIDOMIROV, GM; MALYUCHKOV, OT; YASTREBOV, LI.
CLUSTER MODEL OF HYDROGEN INTERACTION WITH TRANSITION-METALS
ZHURNAL FIZICHESKOI KHIMII 57(5), 1198-1203 (1983)

322. POPOVA, NV; ZHIDOMIROV, GM; KATSNELSON, AA; YASTREBOV, LI.
CLUSTERS IN ALLOYED CATALYSTS ON THE BASIS OF NICKEL
ZHURNAL FIZICHESKOI KHIMII 57(5), 1204-1207 (1983)

323. EVDOKIMENKO, OA; ZHIDOMIROV, GM; MALYUCHKOV, OT; SHPOTIN, IS; YASTREBOV, LI.
CHANGE OF ENERGY THERMS OF CATALYSTS DURING TEMPERATURE RISE
ZHURNAL FIZICHESKOI KHIMII 57(5), 1208-1211 (1983)

324. GRITSENKO, OV; BAGATURIANTS, AA; ZHIDOMIROV, GM; KAZANSKII, VB.
ON THE USE OF FREE ELECTRON-GAS APPROXIMATION FOR THE ESTIMATION OF MULTIELECTRON SYSTEM CORRELATION-ENERGY
DOKLADY AKADEMII NAUK SSSR 265(5), 1166-1169 (1982)

325. PELMENSHCHIKOV, AG; ZHIDOMIROV, GM; ZAMARAEV, KI.
COMPARATIVE QUANTUM-CHEMICAL STUDIES OF PROTON-DONATING CENTERS OF ALUMINOSILICATES
REACTION KINETICS AND CATALYSIS LETTERS 21(1-2), 115-120 (1982)
326. ANIKIN, NA; BAGATURYANTS, AA; ZHIDOMIROV, GM; KAZANSKII, VB.
NON-EMPIRICAL CALCULATION OF THE REACTION OF METHANE WITH PALLADIUM ATOMS
ZHURNAL FIZICHESKOI KHIMII 56(12), 3003-3007 (1982)
327. BAGATURYANTS, AA; ANIKIN, NA; ZHIDOMIROV, GM; KAZANSKII, VB.
NON-EMPIRICAL CALCULATION OF THE REACTION PATTERN OF THE H-2 DISSOCIATION ADDITION TO PD ATOMS
ZHURNAL FIZICHESKOI KHIMII 56(12), 3017-3022 (1982)
328. GORB, LG; ZHIDOMIROV, GM; ABRONIN, IA.
QUANTUM-CHEMICAL INVESTIGATION OF THE EFFECT OF THE SOLVENT ON THE ELECTRONIC-STRUCTURE AND REACTIVITY OF MOLECULES .4. EFFECT OF IONIC ASSOCIATION AND THE DIELECTRIC CONTINUUM ON THE ENERGETICS OF A 1,2-PROTON SHIFT
BULLETIN OF THE ACADEMY OF SCIENCES OF THE USSR DIVISION OF CHEMICAL SCIENCE 31(12), 2341-2347 (1982)
329. KOKOREV, VN; VYSHINSKII, NN; MASLENNIKOV, VP; ABRONIN, IA; ZHIDOMIROV, GM; ALEKSANDROV, YA.
ELECTRONIC-STRUCTURE AND CHEMICAL CONVERSIONS OF PEROXIDES .2. MINDO/3 CALCULATIONS OF REACTION-MECHANISM IN NON-CATALYTIC EPOXIDATION OF OLEFINS BY HYDROPEROXIDES
JOURNAL OF STRUCTURAL CHEMISTRY 23(6), 830-837 (1982)
330. SENCHENYA, IN; MIKHEIKIN, ID; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATIONS OF CHEMISORPTION AND ELEMENTARY ACTS OF CATALYTIC REACTIONS WITHIN THE FRAMEWORK OF A CLUSTER MODEL .8. INTERACTION OF WATER-MOLECULES WITH SILICA-GEL AND H-FORMS OF ZEOLITES
KINETICS AND CATALYSIS 23(3), 496-501 (1982)
331. EVDOKIMENKO, OA; ZHIDOMIROV, GM; YASTREBOV, LI.
ELECTRON T-MATRIX TEMPERATURE-DEPENDENCE IN CRYSTALS
FIZIKA TVERDOGO TELA 24(3), 657-662 (1982)
332. STEPANYUK, VS; ZHIDOMIROV, GM; KATSNELSON, AA; SHPOTIN, IS; YASTREBOV, LI.
INTER-ATOMIC INTERACTION POTENTIAL WITHIN THE FRAMEWORK OF A PHASE-SHIFT METHOD
ZHURNAL FIZICHESKOI KHIMII 56(1), 124-128 (1982)
333. CHUVYLKIN, ND; ZHIDOMIROV, GM.
PRINCIPLES FOR SELECTION AND QUANTUM-CHEMICAL ANALYSIS OF MINIMUM SURFACE COMPLEXES IN CLUSTER-METHODS
ZHURNAL FIZICHESKOI KHIMII 55(1), 1-11 (1981)
334. ANIKIN, NA; BAGATURYANTS, AA; ZHIDOMIROV, GM; KAZANSKII, VB.
USE OF SSP MO LCAO METHOD FOR NON-EMPIRICAL CALCULATION OF MOLECULAR REACTION WITH PALLADIUM ATOM
ZHURNAL FIZICHESKOI KHIMII 55(8), 2030-2034 (1981)
335. BAGATURYANTS, AA; ANIKIN, NA; ZHIDOMIROV, GM; KAZANSKII, VB.
NON-EMPIRICAL CALCULATION OF MOLECULAR-HYDROGEN REACTION WITH PALLADIUM ATOM
ZHURNAL FIZICHESKOI KHIMII 55(8), 2035-2039 (1981)
336. BAGATURYANTS, AA; KUZMINSKII, MB; ZHIDOMIROV, GM.
SUCCESSIVE APPROACH TO THE PREPARATION OF A MODEL POTENTIAL FOR VALENT ELECTRONS
ZHURNAL FIZICHESKOI KHIMII 55(11), 2752-2758 (1981)
337. ABRONIN, IA; BELENKII, LI; ZHIDOMIROV, GM; GOLDFARB, YL.
CORRELATION OF ACTIVITY AND SELECTIVITY IN ELECTROPHILIC SUBSTITUTION-REACTIONS OF 5-MEMBERED HETEROAROMATIC-COMPOUNDS .2. QUANTUM-CHEMICAL STUDY OF THE INFLUENCE OF ELECTROPHILIC AGENT NATURE
ZHURNAL ORGANICHESKOI KHIMII 17(6), 1134-1139 (1981)
338. PELMENSHCHIKOV, AG; MIKHEIKIN, ID; ZHIDOMIROV, GM.
CLUSTER SCHEME FOR THE QUANTUM-CHEMICAL CALCULATION OF SURFACE-STRUCTURES IN THE FRAMEWORK OF THE MINDO/3 METHOD
KINETICS AND CATALYSIS 22(6), 1132-1135 (1981)
339. SENCHENYA, IN; MIKHEIKIN, ID; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATIONS OF CHEMISORPTION AND THE ELEMENTARY ACTS OF CATALYTIC REACTIONS WITHIN THE FRAMEWORK OF A CLUSTER MODEL .12. INTERACTION OF NH3 WITH SILICA-GEL AND THE H FORMS OF

ZEOLITES
KINETICS AND CATALYSIS 22(5), 915-920 (1981)

340. ABRONIN, IA; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL STUDY OF THE INFLUENCE OF THE SOLVENT ON THE ELECTRONIC-STRUCTURE AND REACTIVITY OF MOLECULES .3. 1,2-PROTON SHIFT IN PROTONATED BENZENE
BULLETIN OF THE ACADEMY OF SCIENCES OF THE USSR DIVISION OF CHEMICAL SCIENCE 30(8), 1422-1426 (1981)

341. KOKOREV, VN; VYSHINSKII, NN; MASLENNIKOV, VP; ABRONIN, IA; ZHIDOMIROV, GM; ALEKSANDROV, YA.
ELECTRONIC-STRUCTURE AND CHEMICAL TRANS-FORMATIONS OF PEROXIDES .1. MINDO-3 CALCULATIONS OF THE GEOMETRY AND THE ENTHALPIES OF FORMATION OF THE GROUND-STATE OF ORGANIC AND HETEROORGANIC PEROXIDES
JOURNAL OF STRUCTURAL CHEMISTRY 22(4), 485-491 (1981)

342. KORSUNOV, VA; CHUVYLKIN, ND; ZHIDOMIROV, GM; KAZANSKII, VB.
SEMI-EMPIRICAL QUANTUM-CHEMICAL CALCULATIONS OF THE INTERMEDIATE COMPLEXES IN CATALYTIC REACTIONS .13. CHEMISORPTION OF ETHANOL ON GAMM-A12O3
KINETICS AND CATALYSIS 22(4), 725-730 (1981)

343. GRITSENKO, OV; BAGATURYANTS, AA; ZHIDOMIROV, GM.
METHOD OF APPROXIMATE NATURAL ORBITALS
JOURNAL OF STRUCTURAL CHEMISTRY 22(3), 429-431 (1981)

344. GAGARIN, SG; ZHIDOMIROV, GM; PLEKHANOV, YV; SENCHENYA, IN.
A QUANTUM-CHEMICAL STUDY OF THE ENERGY-SPECTRUM OF CATALYST SURFACES .3. THE ELECTRONIC-STRUCTURE OF A MODEL ELECTRON-ACCEPTOR CENTER OF THE SIO2 SURFACE
JOURNAL OF STRUCTURAL CHEMISTRY 22(2), 156-161 (1981)

345. SHPOTIN, IS; ZHIDOMIROV, GM; MALYUCHKOV, OT; YASTREBOV, LI.
ELECTRON-STRUCTURE OF NONSTOICHIOMETRIC NICKEL AND PALLADIUM HYDRIDES
FIZIKA METALLOV I METALLOVEDENIE 51(3), 473-479 (1981)

346. KOKOREV, V. N.; VYSHINSKII, N. N.; MASLENNIKOV, V. P.; ABRONIN, I. A.; ZHIDOMIROV, G. M.; ALEKSANDROV, YU.A..
ELECTRONIC STRUCTURE AND CHEMICAL REACTIONS OF PEROXIDES: I. MINDO/3 CALCULATION OF THE GEOMETRY AND ENTHALPY OF FORMATION OF THE GROUND STATES OF ORGANIC AND ORGANOELEMENT PEROXIDES
ZHURNAL STRUKTURNOI KHIMII 22(4), 9 (1981)

347. VYSHINSKII, NN; KOKOREV, VN; KULIKOVA, GP; ABRONIN, IA; ALEXANDROV, IA; ZHIDOMIROV, GM; MASLENNIKOV, VP.
QUANTUM-CHEMICAL CALCULATION OF THE DISASSOCIATION ENERGY OF HOMONUCLEAR BONDS IN ORGANIC PEROXIDES AND HYDRAZINES
DOKLADY AKADEMII NAUK SSSR 250(5), 1140-1144 (1980)

348. ABRONIN, IA; LITVINOV, VP; ZHIDOMIROV, GM; DZHUMANAZAROVA, AZ; GOLDFARB, YL.
CONDENSED HETEROCYCLES .39. QUANTUM-CHEMICAL CALCULATIONS OF REACTIVITY OF SOME CONDENSED S-HETEROCYCLES AND SE-HETEROCYCLES
KHIMIYA GETEROTSIKLICHESKIKH SOEDINENII (2), 199-202 (1980)

349. ABRONIN, IA; CHERKASOV, AV; ZHIDOMIROV, GM.
QUANTUM CHEMICAL STUDY OF INFLUENCE OF SOLVENT ON ELECTRONIC-STRUCTURE AND REACTIVITY OF MOLECULES - AROMATIC ELECTROPHILIC SUBSTITUTION
ZHURNAL FIZICHESKOI KHIMII 54(7), 1888-1890 (1980)

350. SHPOTIN, IS; ZHIDOMIROV, GM; MALYUCHKOV, OT; YASTREBOV, LI.
CLUSTER MODEL FOR THE STRUCTURE OF NONSTOICHIOMETRIC HYDRIDES OF TRANSITION-METALS
ZHURNAL FIZICHESKOI KHIMII 54(11), 2739-2744 (1980)

351. BAGATURYANTS, AA; GRITSENKO, OV; ZHIDOMIROV, GM.
INTERACTION OF DIFFUSIVE AND LOCALIZED ORBITALS
ZHURNAL FIZICHESKOI KHIMII 54(12), 2993-3000 (1980)

352. SENCHENYA, IN; MIKHEIKIN, ID; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATIONS OF CHEMISORPTION AND THE ELEMENTARY ACTS OF CATALYTIC REACTIONS WITHIN THE FRAMEWORK OF A CLUSTER MODEL .11. DEHYDRATION OF ETHYL-ALCOHOL
KINETICS AND CATALYSIS 21(5), 851-855 (1980)

353. GRITSENKO, OV; BAGATURYANTS, AA; ZHIDOMIROV, GM.
A NEW LOCAL APPROXIMATION OF THE HARTREE-FOCK EXCHANGE POTENTIAL

JOURNAL OF STRUCTURAL CHEMISTRY 21(3), 272-276 (1980)

354. ABRONIN, IA; BURSHTEIN, KY; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL CALCULATIONS OF SOLVENT EFFECTS ON THE ELECTRONIC-STRUCTURE AND REACTIVITY OF MOLECULES
JOURNAL OF STRUCTURAL CHEMISTRY 21(2), 236-255 (1980)

355. KORSUNOV, VA; CHUVYLKIN, ND; ZHIDOMIROV, GM; KAZANSKII, VB.
COMPARISON OF IONIC AND COVALENT SCHEMES FOR ACCOUNTING FOR CRYSTAL-CHEMICAL ENVIRONMENT OF ACTIVE-CENTERS ON OXIDES
KINETICS AND CATALYSIS 21(2), 311-315 (1980)

356. ABRONIN, IA; ZAGRADNIK, R; ZHIDOMIROV, GM.
SCF-MO LCAO CALCULATIONS OF THE POTENTIAL HYPERSURFACE OF H2CLIF IN THE SINGLET AND LOWER TRIPLET-STATES
JOURNAL OF STRUCTURAL CHEMISTRY 21(1), 1-5 (1980)

357. CHYVYLKIN, ND; ZHIDOMIROV, GM; KAZANSKII, VB.
SEMI-EMPIRICAL QUANTUM-CHEMICAL CALCULATIONS OF INTERMEDIATE COMPLEXES IN CATALYTIC REACTIONS .12. REACTION BETWEEN C2H4 AND O- ON MGO
KINETICS AND CATALYSIS 20(1), 202 (1979)

358. DZHUMANAZAROVA, AZ; ABRONIN, IA; LITVINOV, VP; ZHIDOMIROV, GM; KORSUNOV, VA.
QUANTUM-CHEMICAL CALCULATIONS OF DONOR-ACCEPTOR COMPLEXES OF TETRACYANOETHYLENE WITH 5-MEMBER AROMATIC HETEROCYCLES
KHIMIYA GETEROTSIKLICHESKIKH SOEDINENII (11), 1456 (1979)

359. BAGATURYANTS, AA; KORSUNOV, VA; CHUVYLKIN, ND; ZHIDOMIROV, GM.
PRIME ALGORITHM, GUARANTEEING THE CONVERGENCE OF SOLUTION OF SSP MO LCAO EQUATIONS FOR CLOSED ELECTRON SHELLS
ZHURNAL FIZICHESKOI KHIMII 53(9), 2340 (1979)

360. ZHIDOMIROV, G. M.; BAGATURYANTS, A. A.; ABRONIN, I. A..
APPLIED QUANTUM CHEMISTRY
PUBLISHER: KHIMIYA, MOSCOW , (1979)

361. MIKHEIKIN, ID; LUMPOV, AI; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATIONS OF CHEMISORPTION AND ELEMENTARY ACTS OF CATALYTIC REACTIONS WITHIN THE FRAMEWORK OF THE CLUSTER MODEL .4. PROPERTIES OF SURFACE BRIDGE OH GROUPS IN ALUMINOSILICATES AND ZEOLITES - INFLUENCE OF SI-A1 RATIO
KINETICS AND CATALYSIS 19(4), 850 (1978)

362. MIKHEIKIN, ID; ABRONIN, IA; ZHIDOMIROV, GM; KAZANSKY, VB.
CLUSTER MODEL CALCULATIONS OF CHEMISORPTION AND ELEMENTARY ACTS OF CATALYTIC REACTIONS .1. ISOTOPIC SUBSTITUTION OF HYDROGEN-ATOMS OF SURFACE OH GROUPS OF SILICA-GEL
JOURNAL OF MOLECULAR CATALYSIS 3(6), 435 (1978)

363. KAZANSKY, VB; GRITSCOV, AM; ANDREEV, VM; ZHIDOMIROV, GM.
SPECTROSCOPIC STUDY OF PROTON-TRANSFER IN HETEROGENEOUS ACIDIC CATALYSIS
JOURNAL OF MOLECULAR CATALYSIS 4(2), 135 (1978)

364. MIKHEIKIN, ID; ABRONIN, IA; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATIONS OF ELECTRONIC-STRUCTURE OF MOLECULES, ADSORBED ON SURFACE OF IONIC-CRYSTALS .4. MODELING ELECTROSTATIC-FIELD OF IONIC-CRYSTALS BY FINITE SET OF COULOMB CENTERS
ZHURNAL FIZICHESKOI KHIMII 52(2), 448 (1978)

365. LUMPOV, AI; MIKHEIKIN, ID; ZHIDOMIROV, GM; KAZANSKII, VB.
INTERPRETATION OF ESR-SPECTRA OF WEAKLY BOUND, LOW-SPIN SURFACE COMPLEXES (CU...O2)2+
KINETICS AND CATALYSIS 19(6), 1265 (1978)

366. ABRONIN, IA; BELENKII, LI; ZHIDOMIROV, GM; GOLDFARB, YL.
STABLE HETEROARENIUM IONS .4. QUANTUM-CHEMICAL CALCULATIONS OF RELATIVE STABILITY OF THIOPHENIUM IONS, CARRYING METHYLMERCAPTO GROUP
ZHURNAL ORGANICHESKOI KHIMII 14(6), 1305 (1978)

367. ABRONIN, IA; ZHIDOMIROV, GM.
ELECTRONIC-STRUCTURE, PHYSICAL-PROPERTIES AND REACTIVITY OF 5-MEMBERED AROMATIC HETEROCYCLES (REVIEW)
KHIMIYA GETEROTSIKLICHESKIKH SOEDINENII (1), 3 (1977)

368. VYSHINSKII, NN; KOKOREV, VN; ABRONIN, IA; ALEXANDROV, IA; ZHIDOMIROV, GM.
QUANTUM-CHEMICAL INVESTIGATION OF MECHANISM OF INITIAL-STAGE OF REACTION OF TRIMETHYLBORON

OXIDATION BY MOLECULAR-OXYGEN
DOKLADY AKADEMII NAUK SSSR 236(4), 883 (1977)

369. CHUVYLKIN, ND; ZHIDOMIROV, GM; KAZANSKY, VB.
S-3(-) RADICALS STABILIZED ON MGO SURFACE
JOURNAL OF MAGNETIC RESONANCE 26(3), 433 (1977)

370. PARMON, VN; KOKORIN, AI; ZHIDOMIROV, GM.
INTERPRETATION OF POLYCRYSTALLINE ESR-SPECTRA OF NITROXIDE BIRADICALS
JOURNAL OF MAGNETIC RESONANCE 28(3), 339 (1977)

371. PARMON, VN; KOKORIN, AI; ZHIDOMIROV, GM.
CONFORMATIONAL STRUCTURE OF NITROXIDE BIRADICALS USE OF BIRADICALS AS SPIN PROBES
JOURNAL OF STRUCTURAL CHEMISTRY 18(1), 104 (1977)

372. ZHIDOMIROV, GM.
SOME METHODS OF APPROACH IN QUANTUM-CHEMICAL THEORY OF HETEROGENEOUS CATALYSIS
KINETICS AND CATALYSIS 18(5), 977 (1977)

373. MIKHEIKIN, ID; ABRONIN, IA; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATIONS OF CHEMISORPTION AND ELEMENTARY ACTS OF CATALYTIC REACTIONS IN FRAMEWORK OF CLUSTER MODEL .2. PROPERTIES OF SURFACE OH GROUPS OF OXIDES
KINETICS AND CATALYSIS 18(6), 1295 (1977)

374. CHUVYLKIN, ND; ZHIDOMIROV, GM; KAZANSKY, VB.
SEMIEMPIRICAL QUANTUM CHEMICAL CALCULATIONS OF INTERMEDIATE COMPLEXES IN CATALYTIC REACTIONS .7. BUTENE ISOMERIZATION OVER BASIC CATALYSTS
JOURNAL OF CATALYSIS 44(1), 76 (1976)

375. PARMON, VN; ZHIDOMIROV, GM.
CALCULATION OF ESR-SPECTRUM OF A DYNAMIC BIRADICAL SYSTEM WITH MORE THAN 2 CONFORMATIONS
MOLECULAR PHYSICS 32(3), 613 (1976)

376. MIKHEIKIN, I.D.; ZHIDOMIROV, G.M..
AVERAGING OF MAGNETIC-RESONANCE SPECTRA IN THE CASE OF QUANTUM FINITE MOTION WITH LARGE AMPLITUDE
THEORETICAL AND EXPERIMENTAL CHEMISTRY 12(2), 192 (1976)

377. MUROMTSEV, V.I.; SHTEINSHNEIDER, N.YA.; SAFRONOV, S.N.; GOLIKOV, V.P.; KUZNETSOV, A.I.; ZHIDOMIROV, G.M..
SPIN-LATTICE RELAXATION OF IMINOXYL RADICALS IN FROZEN SOLUTIONS
SOVIET PHYSICS - SOLID STATE 17(3), 517 (1976)

378. KAZANSKY, VB; BOROVKOV, VY; ZHIDOMIROV, GM.
NUCLEAR MAGNETIC-RESONANCE STUDIES OF COMPLEXES FORMED BY ADSORBED MOLECULES AND TETRAHEDRAL CO2+ AND NI2+ IONS
JOURNAL OF CATALYSIS 39(2), 205 (1975)

379. MIKHEIKIN, ID; ABRONIN, IA; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATIONS OF ELECTRONIC-STRUCTURE OF MOLECULES ADSORBED ON SURFACE OF ION CRYSTALS
ZHURNAL FIZICHESKOI KHIMII 49(5), 1306 (1975)

380. MUROMTSEV, VI; SHTEINSHNEIDER, NY; SAFRONOV, SN; GOLIKOV, VP; KUZNETSOV, AI; ZHIDOMIROV, GM.
SPIN-LATTICE RELAXATION OF AMINOXYL RADICALS IN FROZEN SOLUTIONS
FIZIKA TVERDOGO TELA 17(3), 813 (1975)

381. CHUVYLKIN, ND; ZHIDOMIROV, GM; UMANSKY, IM.
INDO CALCULATIONS OF N2-3 AND N-4 FREE-RADICALS
CHEMICAL PHYSICS LETTERS 33(3), 576 (1975)

382. CHUVYLKIN, ND; ZHIDOMIROV, GM; KAZANSKY, VB.
SEMIEMPIRICAL QUANTUM CHEMICAL CALCULATIONS OF INTERMEDIATE COMPLEXES IN CATALYTIC REACTIONS .6. BUTENE ISOMERIZATION
JOURNAL OF CATALYSIS 38(1-3), 214 (1975)

383. PARMON, VN; KOKORIN, AI; ZHIDOMIROV, GM; ZAMARAEV, KI.
MECHANISM OF SPIN EXCHANGE IN LONG-CHAIN NITROXIDE BIRADICALS
MOLECULAR PHYSICS 30(3), 695 (1975)

384. ZHIDOMIROV, GM; KABANKIN, AS.
STRUCTURE OF COMPLEXES OF RADICALS WITH ORGANIC LIGANDS .2. CNDO CALCULATIONS OF G-TENSORS
JOURNAL OF MAGNETIC RESONANCE 19(1), 47 (1975)

385. ZHIDOMIROV, GM; ABRONIN, IA; MICHEIKIN, ID; CHUVYLKIN, ND.

CALCULATION OF ISOTROPIC HYPERFINE COUPLING-CONSTANTS IN CYCLOBUTYL RADICAL
JOURNAL OF MAGNETIC RESONANCE 17(2), 161 (1975)

386. ABRONIN, I.A.; ZHIDOMIROV, G.M..
QUANTUM-CHEMICAL CALCULATIONS OF SPIN DENSITY DISTRIBUTION IN SATURATED ALIPHATIC SYSTEMS
FIZIKA MOLEKUL (1), 47 (1975)

387. GOLDFARB, YL; LITVINOV, VP; ZHIDOMIROV, GM; ABRONIN, IA; ZAKHARYAN, RZ.
STUDIES IN SERIES OF CONDENSED HETEROAROMATIC SYSTEMS INCLUDING THIOPHENE RING .24. QUANTUM CHEMICAL-ANALYSIS OF ISOMERIC THIENOTHIOPHENES REACTIVITY IN ELECTROPHILIC SUBSTITUTION-REACTIONS
CHEMICA SCRIPTA 5(2), 49 (1974)

388. PARMON, VN; ZHIDOMIROV, GM.
CALCULATION OF ESR-SPECTRUM SHAPE OF DYNAMIC BIRADICAL SYSTEM
MOLECULAR PHYSICS 27(2), 367 (1974)

389. CHUVYLKI.ND; ZHIDOMIR.GM; KAZANSKY, VB.
ESR PARAMETERS OF CO+ RADICALS ON A H-Y-TYPE ZEOLITE
CHEMICAL PHYSICS LETTERS 26(2), 180 (1974)

390. MIKHEIKIN, ID; ZHIDOMIROV, GM; CHUVYLKIN, ND; KAZANSKII, VB.
PARAMETERS OF ESR-SPECTRA AND STRUCTURE OF O3-RADICALS
JOURNAL OF STRUCTURAL CHEMISTRY 15(5), 678 (1974)

391. MIKHEIKIN, ID; ZHIDOMIROV, GM; KAZANSKII, VB.
CALCULATION OF ELECTRONIC-STRUCTURE OF MOLECULES, ADSORBED ON IONIC-CRYSTAL SURFACE .1. ESTIMATION OF ELECTROSTATIC INTERACTIONS
ZHURNAL FIZICHESKOI KHIMII 48(12), 2920 (1974)

392. BROTIKOVSKII, O. I.; ZHIDOMIROV, G. M.; KAZANSKII, V. B..
QUANTUM EFFECTS OF ANISOTROPIC ROTATION IN THE ESR OF THE METHYL RADICAL
THEOR. EXP. CHEM. 8, 653 (1974)

393. CHUVYLKIN, ND; ZHIDOMIROV, GM.
CNDO-SP CALCULATION OF G-TENSORS OF FREE-RADICALS
MOLECULAR PHYSICS 25(5), 1233 (1973)

394. CHUVYLKIN, ND; ZHIDOMIROV, GM.
CALCULATIONS OF ANISOTROPIC HYPERFINE COUPLING-CONSTANTS IN FREE-RADICALS
JOURNAL OF MAGNETIC RESONANCE 11(3), 367 (1973)

395. PARMON, VN; KOKORIN, AI; ZHIDOMIROV, GM; ZAMARAEV, KI.
EVIDENCE FOR SLOW EXCHANGE IN ESR-SPECTRA OF NITROXIDE BIRADICALS
MOLECULAR PHYSICS 26(6), 1565 (1973)

396. ZHIDOMIROV, GM; CHUVYLKIN, ND.
CALCULATIONS OF ISOTROPIC HYPERFINE COUPLING-CONSTANTS IN FREE-RADICALS
THEORETICA CHIMICA ACTA 30(2), 197 (1973)

397. ZHIDOMIROV, GM; ABRONIN, IA.
CNDO/SP CALCULATION OF SPIN-SPIN COUPLING-CONSTANTS J13CH IN C6H7 CATION
CHEMICAL PHYSICS LETTERS 21(2), 409 (1973)

398. CHUVYLKIN, ND; SCHASTNEV, PV; ZHIDOMIROV, GM.
CALCULATION OF PROTON-PROTON COUPLING BY PI-ELECTRONS
MOLECULAR PHYSICS 23(3), 639 (1972)

399. ZHIDOMIROV, GM; CHUVYLKIN, ND.
CALCULATION OF HYPERFINE COUPLING-CONSTANTS IN FREE-RADICALS
CHEMISTRY AND PHYSICS OF LIPIDS 14(1), 52 (1972)

400. SHTEINSHNEIDER, NY; ZAMARAEV, KI; ZHIDOMIROV, GM.
APPLICATION OF COMPUTER FOR ANALYSIS OF ELECTRON-PARAMAGNETIC RESONANCE SPECTRA OF CU(II) COMPOUNDS IN POLYCRYSTALS AND GLASSES
ZHURNAL STRUKTURNOI KHIMII 13(5), 795 (1972)

401. CHUVYLKIN, ND; ZHIDOMIROV, GM.
ESR-SPECTRA OF MATRIX-STABILIZED HYDRONIUM RADICALS H3O AND D3O
CHEMISTRY AND PHYSICS OF LIPIDS 14(1), 70 (1972)

402. MUROMTSEV, V.I.; POMORTSEV, V.V.; SAFRONOV, S.N.; GOLIKOV, V.P.; KLINSHPONT, E.R.; MILINCHUK, V.K.; ZHIDOMIROV, G.M..
ROLE OF ELECTRON-NUCLEAR INTERACTIONS IN EPR RELAXATION PROCESSES IN SOLIDS

FIZIKA TVERDOGO TELA 13(4), 1062 (1971)

403. ZHIDOMIROV, G.M.; SALIKHOV, K.M..
MODULATION EFFECTS IN FREE-RADICAL SPIN-ECHO SIGNALS
THEOR. EXP. CHEM. 4, 332 (1971)

404. GILINSKAYA, L. G.; ZHIDOMIROV, G. M.; SHCHERBAKOVA, M.YA; BRODSKII, A. I..
PARAMAGNETIC DEFECT CENTERS PO2-3IN APATITE
PUBLISHER: NAUKOVA DUMKA, KIEV , 69 (1970)

405. BAZHIN, NM; SCHASTNE.PV; CHUVYLKI.ND; BERDNIKO.VM; FEDOROV, VK; MERKULOV, AP; SHTEINGA.VD.
ELECTRON PROTON RESONANCE SPECTRA OF FLUORINE-CONTAINING PHENOXYL RADICALS
ZHURNAL STRUKTURNOI KHIMII 11(6), 998 (1970)

406. POMORTSEV, V.V.; SAFRONOVA, U.I.; ZHIDOMIROV, G.M..
PHASE RELAXATION IN A TWO-SPIN SYSTEM DUE TO THE SPIN-LATTICE INTERACTION
FIZIKA TVERDOGO TELA 12(1), 16 (1970)

407. ZHIDOMIROV, G.M.; SALIKHOV, K.M..
ON THE THEORY OF SPECTRAL DIFFUSION IN MAGNETICALLY DILUTE SOLIDS VERSIONS
ZHURNAL EKSPERIMENTAL'NOI I TEORETICHESKOI FIZIKI 56(6), 1933 (1969)

408. ZHIDOMIROV, GM; SALIKHOV, KM.
CONTRIBUTION TO THEORY OF SPECTRAL DIFFUSION IN MAGNETICALLY DILUTED SOLIDS
SOVIET PHYSICS JETP-USSR 29(6), 1037 (1969)

409. ZHIDOMIROV, GM; SALIKHOV, KM; RAITSIMRING, AM; TSVETKOV, YD.
THE NATURE OF THE BROADENING OF EPR LINES AS DETERMINED BY DIPOLE-DIPOLE INTERACTION IN MAGNETICALLY DILUTED SYSTEMS
J STRUCT CHEM. 10, 15 (1969)

410. ZHIDOMIROV, G. M.; SALIKHOV, K. M; TSVETKOV, YUD; YUDANOV, V. F; RAITSIMRING, A. M.
A STUDY OF THE INTERACTION BETWEEN PARAMAGNETIC SPECIES AND THE MAGNETIC NUCLEI OF THE SURROUNDING MOLECULES BY ELECTRON SPIN ECHO SPECTROSCOPY
J. STRUCT. CHEM 9, 704 (1968)

411. ZHIDOMIROV, G.M.; SCHASTNEV, P.V..
CALCULATION OF THE HYPERFINE INTERACTION OF AN UNPAIRED ELECTRON WITH THE PROTONS IN A STATIONARY METHYL GROUP
THEORETICAL AND EXPERIMENTAL CHEMISTRY 3(4), 319 (1967)

412. ZHIDOMIROV, G. M.; BUCHACHENKO, A. L..
STUDY OF EXCHANGE INTERACTIONS IN POLYRADICAL SYSTEMS BY EPR
J. STRUCT. CHEM. 8, 987 (1967)

413. ZHIDOMIROV, G.M.; SCHASTNEV, P.V..
HYPERFINE INTERACTION OF THE UNPAIRED ELECTRON WITH NUCLEI IN A METHYL GROUP IN PI -ELECTRON RADICALS
TEORETICHESKAYA I EKSPERIMENTAL'NAYA KHIMIYA 1(5), 649 (1965)

414. ZHIDOMIROV, GM; TSVETKOV, YD.
THE POSSIBILITY OF STUDYING THE FREE RADICAL CONFORMATIONS IN SOME ALICYCLIC COMPOUNDS USING THE EPR METHOD
OPTIKA I SPEKTROSKOPIYA 17(1), 67 (1964)

415. KAZANSKII, VB; PARIISKII, GB; ALEKSANDROV, IV; ZHIDOMIROV, GM.
ELECTRON PARAMAGNETIC RESONANCE INVESTIGATION OF THE INTERACTION OF FREE RADICALS WITH THE SURFACE OF A SOLID (SILICA GEL)
SOVIET PHYSICS-SOLID STATE 5(2), 473 (1963)

416. ALEKSANDROV, IV; ZHIDOMIROV, GM.
CALCULATION OF THE SPIN-LATTICE RELAXATION TIME FOR RADICALS IN MOLECULAR CRYSTALS
SOVIET PHYSICS JETP-USSR 14(1), 94 (1962)

417. ALEKSANDROV, I. V.; ZHIDOMIROV, G. M..
SPIN-LATTICE RELAXATION TIME CALCULATION FOR RADICALS IN MOLECULAR CRYSTALS
ZHURNAL EXPER. TIEORET. FIZIKI 41, 127 (1961)

418. RYBAKOV, A.; BRYUKHANOV, I.; LARIN, A.; ZHIDOMIROV, G..
THEORETICAL ASPECTS OFMETHANOL CARBONYLATION ON COPPER-CONTAINING ZEOLITES
PETROL. CHEM 56, (0)