

Георгий Михайлович Жидомиров



(11.07.1933 – 31.07.2019)

Ушел из жизни Георгий Михайлович Жидомиров - известный ученый 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 2003г. 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 1960г. 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. Счастливым 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 1964г. 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 свободных 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 продолжают 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, 1978г. (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, 1980г. (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 становится 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 Бренstedовских 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 1982г., 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 термо-химической 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, ВИНТИ АН СССР), 1984г., т.9 (совместно с И.Д. Михайкиным) 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 непереключаемых (MINDO/3-HB) и переходных элементов (NDDO/MC); расчета магнитно-резонансных параметров спектров ЭПР (Spin-Hamiltonian), электронных спектров ($X\alpha$ -Omega) и спектров XAFS ($X\alpha$ -continuous), расчета формы анизотропно-уширенных спектров ЭПР (ESR1, ESR2, BIRAD); статических и MAS спектров ЯМР квадрупольных ядер (SATRAS).

В последующем цеолиты остаются одним из главных приоритетов в работах Г.М. Жидомирова, однако предметом исследований являются 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 составляет 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 $(Zn-O-Zn)^{2+}$, $(Fe-O-Fe)^{2+}$ 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 бивалентные 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 этих исследований частично представлены в обзорах G.M. Zhidomirov, A.A. Shubin, R.A. van Santen "Structure and Reactivity of Metal Ion 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 возглавляемого им коллектива сотрудников охватывает 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 является членом Совета директоров Международного общества по теоретической химической физике, он заместитель главного редактора «Журнала структурной химии», член редакции журнала «Кинетика и катализ».

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