MOLECULAR DYNAMICS SIMULATIONS OF CHEMICAL PHENOMENA IN CONDENSED PHASES

A.V.Nemukhin* and B.L.Grigorenko

Laboratory of Chemical Cybernetics, Department of Chemistry, M.V.Lomonosov Moscow State University, Moscow, 119899, Russian Federation

We are developing approaches to modeling properties and reactivity of chemical substances in condensed phases by using molecular dynamics simulations with the quantum mechanical potential energy surfaces. In particular, structures and spectra of small molecules and intermolecular complexes trapped in rare-gas clusters have been considered [1-6]. Such systems serve as the models to study matrix isolation phenomena at low temperatures. The potentials are constructed by a combination of *ab initio* quantum chemistry methods and semiemirical quantum-based techniques, like diatomics-in-molecules (DIM). An important feature of this approach is that the many-body contributions to the interaction energy are taken into account. Molecular dynamics simulations on these potential energy surfaces for the ground and excited electronic states allow one to estimate vibrational and electronic spectra of the trapped species. Applications include calculations of electronic properties of lithium clusters inside argon shells [1], vibrational spectra of NBr [2], HF [3], hydrogen fluorine dimer [4] in argon, vibronic spectra of chlorine molecule in neon clusters [5], and SH radical in krypton [6,7].

A novel direction is a development of the combined Quantum Mechanical - Molecular Mechanical (QM/MM) theory for use in simulations of biomolecular systems [8]. At the present stage, the potentials for QM subsystems can be computed at the various *ab initio* levels (Hartree-Fock, multiconfigurational self-consistent field, Moller-Plessett perturbation theory), while the potentials for MM subsystems are described by conventional force field parameters.

[1] B.L.Grigorenko, A.V.Nemukhin, G.B.Sergeev, V.S.Stepanyuk, A.Szasz, Phys.Rev.B., 1994, 50, 18666.
[2] A.V.Nemukhin, B.L.Grigorenko, Chem.Phys.Lett., 1995, 233, 627.
[3] B.L.Grigorenko, A.V.Nemukhin, V.A.Apkarian, J.Chem.Phys., 1996, 104, 5510. [4] A.V.Nemukhin, B.L.Grigorenko, Chem.Phys.Lett., 1997, 270, 103.
[5] B.L.Grigorenko, A.V.Nemukhin, N.V.Ozhegova, Chem.Phys.Lett., 1998, 296, 84.
[6] B.L.Grigorenko, L.Khriachtchev, A.V.Nemukhin, M.Petterson, E.Isoniemi, M.Rasanen, J.Chem.Phys., 1999, 110, 5836.
[7] D.A.Firsov, B.L.Grigorenko, A.V.Nemukhin, L.Khriachtchev, M.Rasanen, Chem.Phys.Lett., 2001, 338, 317.
[8] A.V.Nemukhin, B.L.Grigorenko, A.V.Bochenkova, I.Topol, S.Burt, J.Molec.Struct.(Theochem), 2002, 581, 167.

Phone (095) 939-10-96
Fax (095) 939-02-83
E-mail anem@lcc.chem.msu.ru