MOLECULAR DYNAMICS SIMULATIONS OF CLUSTER FISSION AND FUSION PROCESSES

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We investigate cluster isomer structure and its manifestation in the fission and fusion processes of small atomic clusters using molecular dynamics (MD) methods. The results of MD simulations are compared with those obtained within the jellium approach and in experiment.

We start cluster isomer modelling from the smallest clusters, consisting only of a few atoms, and then add new atoms to the system and minimize the cluster energy on each step [1]. In this way we investigate the cluster fusion process, with the aim to find fusion paths for the most stable and the most symmetric clusters. These simulations explain sequences of magic numbers for noble gas clusters (Ne, Ar, Kr, Xe), which are rather sensitive to the details of electronic and ionic cluster structure. Attention in this calculation is devoted to the role of symmetry (icosahedral, octahedral, dodecahedral, tetrahedral, etc) of small metal clusters in their fusion process and in the formation of their physical properties.

We also report new results of ab-initio all-electrons MD simulations as well as the jellium model calculations of fission barriers for sodium clusters. The MD calculations are performed with the use of the Gaussian 98 software package [2]. We utilize the 6-311G(d) basis set of primitive Gaussian functions to expand the cluster orbitals and the density-functional theory based on the hybrid Becke-type three-parameter exchange functional paired with the gradient-corrected Lee, Yang and Parr correlation functional (B3LYP) [2]. The jellium results are obtained with the use of the two-center deformed jellium model and local-density approximation [3].

The following symmetric (Na102+ → 2Na5+ and Na182+ → 2Na9+), as well as asymmetric (Na102+ → Na11+ + Na1 and Na182+ → Na13+ + Na15+) fission channels are considered. The importance of cluster deformation effects in the fission process is elucidated with the use of the overlapping-spheroids shape parametrization allowing one an independent variation of deformations in the parent and daughter clusters [3].

We investigate the isomer dependence of the fission barriers as well as the barriers for transition between different cluster isomer forms. For this purpose, we consider three different isomers of the parent doubly-charged Na102+ cluster having the ionic structure of distorted tetrahedron (lowest energy state), or characterized by the C4v and D4d point symmetry groups.

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