DYNAMICS OF NANOCLUSTERS - UNDERSTANDING THE STABILITY OF MATTER

ANA PROYKOVA[1]

Abstract

The systems at the nanoscale exhibit extremely complex behavior and because of their finite-size many of the assumptions made in conventional macroscopic physics (such as weak coupling to the environment and disregarding of fluctuations) are not appropriate. Wise developments made computational techniques useful in describing the stability of the objects - at the nanscale and bulk. The cluster stability has been explored both experimentally and theoretically in the past to study temperature driven structural transformation, see [1, 2] It has been found that the translational non-invariance imposes restrictions on the type of interacting potentials useful in modeling stable systems. Result is that stable configurations are due to kinetics. This means that regions of the phase space that are extremely weakly populated in bulk, e.g. the probability of populating them is zero in practice, become favorable for small systems.

More about the structure can be found from the vibrational spectra. The normal modes are computed in the harmonic approximation from the diagonalized Hessian matrix:

$$H = \vec{\nabla}\vec{\nabla}U, \tag{1}$$

where the interaction potential U in molecular clusters contains a Lennard-Jones (short-range) and a Coulomb term (long-range).

The present article presents hints in using techniques like Monte Carlo Methods for describing self-organization of nanoclusters towards stability, which makes them applicable for drug production, see [3].

References

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[1]Faculty of Mathematics and Informatics, Sofia University "St. Kliment Ohridski"
E-mail address: anap@phys.uni-sofia.bg

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