

Alkali Halides Nanotubes: Structure and Stability

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In this talk we report the results of accurate quantum mechanical calculations on some alkali halide (LiF, NaCl, KBr) neutral clusters. The relative stability of $(MX)_{n=2-28}$ structural isomers was studied using DFT (B3LYP/LAVCV3P**). For the members of the cubic and nanotube series Coupled Cluster calculations at the CCSD/SDD level were also performed. Møller-Plesset perturbation theory at the MP2/LAVCV3P** level of calculation was also used to check for possible inconsistencies in the DFT results for the $(MX)_{n=1-10}$ clusters. Quantum dynamics calculations, at room temperature and atmospheric pressure, were also performed for the $(LiF)_{28}$ octagon nanotube. A variety of structures has been found but in this talk we limit the discussion on the tube-like ones. Structural properties and possible mechanisms of formation will be discussed.

The alkali halide nanotubes present much smaller diameters, ranging from 0.241 nm to 0.67 nm (LiF, tetragonal-KBr hexagonal) when compared to the more traditional covalent nanotubes of C (1-2 nm), BN (1-3 nm) or GaN (30-200 nm). This is a consequence of the fact that the interactions are dominantly electrostatic and, therefore, much less strain is involved in making ring-type structures than in the covalent ones.

The results obtained for the $(LiF)_n$ clusters show that overall the cubic series is highly stable as expected from structures which are debris of a crystalline bulk. Surprisingly, however, nanotube clusters with hexagonal and octagonal cross section present similar or higher stability than the corresponding cubic clusters. This result represents a new paradigm for 3D macro assembly of alkali halide clusters. This work was funded by CNPq, FAPERJ and Instituto Nacional de Materiais Complexos Funcionais. F.A.F-L acknowledges support from the National Institute of Health (Grant No. 1K99RR030188-01).