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Evolution of Electronic and Vibrational Polarity of NaF Nanocrystals PHILIP B. ALLEN, CHRISTIAN SCHMIDT[1], SUNY Stony Brook, TUNNA BARUAH, MARK R. PEDERSON, Naval Research Laboratory — Density functional theory is used to study vibrations, electrical dipole moments, and polarizabilities of NaF clusters. We use the NRLMOL code with GGA exchange and correlation, and a large basis set of Gaussian orbitals. Because of prior experimental and theoretical studies, this is a good model system for tracking the evolution of the properties from diatomic molecule to bulk crystal. The predicted ratio of vibrational to electronic contributions to the polarizability increases dramatically with size N in the closed shell clusters Na_NF_N. The open shell system $Na_{14}F_{13}$ has a greatly enhanced electronic polarizability. Contrary to previous studies on this system which treated only the outer electron by quantum mechanics, we find the O_h cubic structure to be stable relative to the polar distorted structures such as C_{3v}. The size of the permanent dipole is predicted to be 2.01 and 5.12 in units ea_B for the C_4v systems Na_9F_9 and $Na_{18}F_{18}$ respectively.

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