

Abstract Submitted
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On the stability and vibrational properties of super-polyiodides

NAICHE JONES, J. ULISES REVELES, SHIV KHANNA, Virginia Commonwealth University — We had earlier shown that a new class of polyhalides can be formed by combining the Al_{13} super-halogen with the conventional halogen, I. Experimental reactivity studies demonstrate that the new super-polyhalides, $\text{Al}_{13}\text{I}_x^-$, exhibit pronounced stability for even numbers of I atoms. Theoretical investigations probing the geometry and the electronic structure reveal that the enhanced stability is associated with pairs of I atoms occupying the on-top sites around the Al_{13}^- core. We had also demonstrated another series, $\text{Al}_{14}\text{I}_x^-$, that exhibits stability for odd numbers of I atoms. In this work we have examined the vibrational properties of the new super-polyiodides using gradient corrected density functionals. It is shown that the low frequency modes involve motion of the central Al and that the geometrical progressions with high iodine coverage can be understood in terms of these vibrations.

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