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Theoretical Study of NaCl and LiCl Clusters BRIDGET ORTIZ, AJIT HIRA, JAMES MCKEOUGH, TED KOETTER, Northern New Mexico College — This research is a Quantum Mechanical study of molecular clusters that examines the chemical properties of small Na_nCl_n and Li_nCl_n clusters (n = 2 - 20). The potentially important role of these molecular species in biochemical and medicinal processes is well known. This work applies the hybrid ab initio methods to derive the different alkali-halide (M_nH_n) geometries. Of particular interest is the competition between hexagonal ring geometries and rock salt structures. Electronic energies, rotational constants, dipole moments, and vibrational frequencies for these geometries are calculated. Magic numbers for cluster stability are identified and are related to the property of cluster compactness. Mapping of the singlet, triplet, and quintet, potential energy surfaces is performed. Calculations were performed to examine the interactions of these clusters with some atoms and molecules of biological interest, including O, O2, and Fe. Potential design of new medicinal drugs is explored. We will also investigate model and material dependence of the results.

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