

5-3-2014

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Recommended Citation

Langholz, Erik; Place, Stephen; Tiessen, John Eric; He, Haiying; and Zygmunt, Stan, "A First-Principle Study of Small Neutral and Anionic Silver Halide Clusters" (2014). *Symposium on Undergraduate Research and Creative Expression (SOURCE)*. 341.
<https://scholar.valpo.edu/cus/341>

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A First-Principle Study of Small Neutral and Anionic Silver Halide Clusters

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Silver halide is a material that was traditionally used in photographic films. In recent years, there has been a revived interest in using small clusters of silver halides for photocatalytic and photovoltaic applications. We present the results of a theoretical study of neutral and anionic Ag_nX_n ($X = \text{F}, \text{Cl}, \text{and Br}$, and $n = 1-6$) clusters. Quantum-mechanical calculations were performed using Density Functional Theory (DFT) in search of the lowest-energy isomers of the neutral and anionic clusters with applied symmetry constraints. The optimal configurations are compared across the series of AgF , AgCl , and AgBr . The variation in binding energies, bond lengths, charge distributions, HOMO-LUMO gaps, and electron affinities will be discussed as a function of cluster size and composition. The study of these clusters allows us to gain a better understanding of the structure and function of these materials in current and future applications.

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John Eric Tiessen is currently a physics major at Valparaiso University. He plans on going to graduate school after completing his undergraduate degree and would like to go into computational work. Stephen Place is a sophomore physics major from Goshen, Indiana. Stephen intends to pursue graduate school after graduation. Erik Langholz is a sophomore mechanical engineering major from Kaiserslautern, Germany. Upon graduating, Erik plans to either become a pilot in the U.S. Air Force or go to graduate school for engineering or applied physics.

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