Density-driven delocalization error for a model solvated electron system STEPHEN DALE, ALBERTO OTERO-DE-LA-ROZA, ERIN JOHNSON, University of California, Merced — Electrides are a unique class of ionic solids in which the anions are replaced by a lone electron localized within a crystal void. Theoretical modeling of these systems is possible using DFT methods. However, delocalization error inherent in common density-functional approximations increases the complexity of this study. To investigate delocalization error effects, we propose a simplified electride model, known in solvated electron chemistry as the Kevan structure. This model localizes an electron within a void formed by six radially-oriented, octahedrally-arranged water molecules. The Kevan structure is then coupled with atoms of various electronegativities, and the resulting complex is used to test different density functionals. We show that fractional charges caused by delocalization error have a significant impact on the electron density of the Kevan structure. Finally, we use results for the Kevan structure to rationalize the calculated band gaps for the actual electrides.

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