Abstract Submitted
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Hybrid functional calculation of Na and K impurities in $CuInSe_2$ and $CuIn_5Se_8$ solar cell materials[1] JANOS KISS, Max Planck Institute for Chemical Physics of Solids Dresden, ELAHEH GHORBANI, Institute of Inorganic and Analytical Chemistry JGU Mainz, HOSSEIN MIRHOSSEINI, Max Planck Institute for Chemical Physics of Solids Dresden, GUIDO ROMA, Service de Recherches de Metallurgie Physique DMN/DEN CEA-Saclay, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids Dresden — Although it is widely known that the presence of Na and K dopants increase the efficiency of $CuIn_xGa_{1-x}Se$ (CIGS) thin film solar cells, the incorporation of these impurities and their effect upon the atomic and electronic structure of the light absorber materials is not yet well understood. Using the HSE06 hybrid functional we studied the structure and energetics of Na and K impurities and also Na-Na, K-K and Na-K dumbbells in different substitutional and interstitial positions in $CuInSe_2$ and $CuIn_5Se_8$ solar cell materials. We found that among substitutional positions, occupying Cu position is energetically more favorable compared to In and Se positions. The interstitial position, where the impurity is tetrahedrally coordinated by four Se atoms is the most stable site to form Na or K interstitials in $CuInSe_2$, wheres in $CuIn_5Se_8$ the pristine copper vacancy positions are more stable. Our data show, that Na-Na, Na-K and K-K dumbbells can form both in $CuInSe_2$ and in $CuIn_5Se_8$ as well. Comparing the formation energy of various dumbbell configurations, creating dumbbells in a pristine vacant copper site in $CuIn_5Se_8$ has the highest association energy between the impurities.

[1]comCIGS I (No. 0327665A) and comCIGS II (No. 0325448C).

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