Light Si Based Clathrates For Thermal Energy Conversion: A First Principles Study\(^1\) YUPING HE, FAN SUI, SUSAN KAULZARICH, GIULIA GALLI, UC Davis — Clathrates containing light, earth abundant elements, i.e. Si and Al, are promising materials for thermoelectric applications, due to their low thermal conductivity, about 2 orders of magnitude smaller than that of bulk Si. However existing Si based clathrates \([1]\) have poor electronic properties for efficient thermal energy conversion. We carried out density functional theory calculations to investigate the electronic and vibrational properties of newly synthesized type I clathrate K\(_8\)Al\(_8\)Si\(_{38}\)\(^2\). We predicted that while Al site occupancy does not substantially affect the structure of these systems, it has a strong influence on their electronic and optical properties. In particular, Al occupancy greatly influences the location of the K atoms, and the magnitude and character of the electronic gap of the clathrate (e.g. Whether direct or indirect). Our findings suggest that K\(_8\)Al\(_8\)Si\(_{38}\) may have much improved electronic properties, compared to several families of clathrates \([2]\) investigated in the recent literature.

\(^2\)F. Sui et al. Synthesis and characterization of type I clathrate K\(_8\)Al\(_8\)Si\(_{38}\) for thermoelectric application (in preparation)

\(^1\)Work supported by DOE-BES under Grant No. DE-FG02-06ER46262 and DOE-Scidac-e under Grant No. DE-FC02-06ER25777.

Yuping He
UC Davis