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**Light Si Based Clathrates For Thermal Energy Conversion: A First Principles Study**[1] YUPING HE, FAN SUI, SUSAN KAUZLARICH, GIULIA GALLI, UC Davis — Clathrates containing light, earth abundant elements, i.e. Si and Al, are promising materilas 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 $K_8Al_8Si_{38}$[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 $K_8Al_8Si_{38}$ may have much improved electronic properties, compared to several families of clathrates [2] investigated in the recent literature.

[1] C. L. Condron et al. Inorg. Chem. 2008, 47, 8204.
[2] F. Sui et al. Synthesis and characterization of type I clathrate $K_8Al_8Si_{38}$ for thermoelectric application (in preparation)

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