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Electronic and structural properties of superionic Cu_2Se from density functional theory[1] MIKAEL RÅSANDER, LARS BERGQVIST, ANNA DELIN, KTH - Royal Institute of Technology — The superionic high temperature phase of Cu_2Se has been found to yield high thermoelectric efficiency due to an interesting combination of low thermal conductivity and a rather high power factor. The low thermal conductivity has been found to be due to the quasi-liquid behaviour of the superionic Cu atoms (Liu et al., Nature Materials, **11**, 422-425 (2012)). Here we will present results obtained using density functional theory calculations of the electronic and structural properties of the superionic Cu_2Se phase. We will especially address how the inclusion of non-local exchange by the use of hybrid density functionals as well as how localization of the Cu 3d-states affect the electronic structure of Cu_2Se.

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