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Novel Rattling Dynamics Explain Low Thermal Conductivity in Aluminium-Doped Potassium Tungstate Defect Pyrochlore

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Abstract content
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In a recent study, we reported an unusual quasielastic inelastic neutron scattering (INS) signal in the K analogue of the Al-doped series of cage compounds with the β-pyrochlore structure, AAl0.33W1.67O6 (A = K, Rb, Cs) [1]. We are studying this family of compounds because the rattling modes of the alkali metal atoms [2, 3] are similar to those found to enhance thermoelectric performance in both clathrates [4] and skutterudites [5]. This talk will discuss our recent thermal conductivity [6] and specific heat data in terms of the vibrational density of states calculated from ab initio molecular dynamics (MD) simulations validated against experimental INS spectra and show the significance of the novel K dynamics for these properties. I will conclude with a tentative sketch of the prospects of these compounds for thermoelectric development.

References
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Apply to be
 considered for a student
   award (Yes / No)?

No

Level for award
 (Hons, MSc,
   PhD)?

No

Main supervisor (name and email)
and his / her institution

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**Would you like to
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No

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