Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **4353** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Metallic bonding in close-packed solids

Tuesday 28 May 2024 14:45 (15 minutes)

We may expect lithium to be the simplest metal as it has only a single $2s$ valence electron. Surprisingly, lithium's crystal structure at low temperature and ambient pressure has long been a matter of debate. In 1984, A. W. Overhauser proposed a rhombohedral $9R$ structure. Subsequent neutron experiments by Schwarz *et al.* in 1990 favour a disordered polytope. More recently, in 2017, Elatresh *et al.* argued against the $9R$ structure while Ackland *et al.* found fcc ordering. In this work, we seek to understand the physical principles that could lead to such conflicting findings. We describe metallic bonding in an arbitrary close-packed structure within the tight-binding approximation. Close-packed structures, also called Barlow stackings, are infinite in number. They can be codified by stacking sequence (*e.g.* fcc $\leftrightarrow ABC$) or by a Hagg code (*e.g.* fcc $\leftrightarrow +++$). From the point of view of an atomic orbital, all close-packed structures offer similar local environments with the same number of nearest neighbours. When hoppings are short-ranged, the tight binding description shows a surprising gauge-like symmetry. As a result, the electronic spectrum is precisely the same for every close-packed structure. This results in competition across a large class of structures that all have the same binding energy.
A preference for one ordering pattern can only emerge from (a) long-ranged (third-neighbour and further) hoppings or (b) phonon free energies at finite temperatures. Our results could explain the observed fcc structure in lithium under high pressure.

Keyword-1

tight-binding

Keyword-2

crystal-structure

Keyword-3

lithium

Author: HE, Eric (University of California, Berkeley)

Co-authors: WILSON, Connor; RAMACHANDRAN, Ganesh

Presenter: WILSON, Connor

Session Classification: (DCMMP) T2-7 Material Properties | Propriétés des matériaux (DPMCM)

Track Classification: Technical Sessions / Sessions techniques: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)