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Pudding mold type band as the origin of large thermopower in $LiRh_2O_4$[1]

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To calculate thermodynamic and transport properties we employ the combination of local density approximation and dynamical mean field theory (LDA+DMFT method.) After a briefly introducing this method, we will focus on the newly synthesized mixed-valent spinel $LiRh_2O_4$ for which a large thermopower is observed in the metallic cubic phase above 230K [1]. We calculate the Seebeck coefficient by LDA+DMFT; not only LDA+DMFT but also by the less involved Boltzmann equation approach well reproduces the experimental values. A careful analysis of the latter shows unexpectedly that the origin of the large thermopower shares a common root with a very different oxide: Na_xCoO_2. We also discuss how it is possible to further increase the powerfactor of $LiRh_2O_4$ through doping, which makes the material even more promoising for technological applications.

[1] Okamoto *et al.* (arXiv:0806.2504)

[1] In cooperation with R. Arita, K. Kuroki, A. V. Lukoyanov, S. Skornyakov, and V.I. Anisimov