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LiNi02 as a high-entropy functional material

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Abstract:

The 2015 discovery of entropy-stabilized transition-metal oxides, such as Mgo.2Coo.2Nio.2Cuo.2Zno.20, [2] has opened a new avenue for synthesizing materials with versatile and highly tunable properties [3]. It only took a few years to realize that such systems can find diverse technological applications, including but not limited to energy storage and catalysis [4]. While the on-going research in the field is currently focused more on exploiting chemical disorder, I will discuss the surprising possibility of high-entropy physics in a prototypical battery cathode material LiNi02, which is nominally pure in terms of its chemical composition. Based on both experimental evidence and our electronic structure theoretical calculations, I will argue that LiNi02 presents a rare example of an electronically disordered system, with contributing spin, charge, and orbital degrees of freedom on nickel as well as oxygen ions. In the light of the aforementioned stabilizing effect of entropy in functional materials, our findings explain the outstanding functional characteristics of LiNi02, as compared to similar cathode materials. The LiNi02 story showcases how insights from fundamental solidstate physics research can help advance technology.

[1] "LiNi02 as a high-entropy charge- and bond-disproportionated glass", Kateryna Foyevtsova, Ilya Elfimov, Joerg Rottier, and George A. Sawatzky, Phys. Rev. 8 100, 165104 (2019).
[2o "Entropy-stabilized oxides", C. M. Rost et al., Nat. Commun. 6, 8485 (2015).
[3o "Order emerging from disorder", Nita Dragoe and David Berardan, Science 366, 573-574 (2019).
[4] "High-entropy energy materials: challenges and new opportunities", Y. Ma et al., Energy Environ. Sci. (2021).

Speaker's Bio:

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