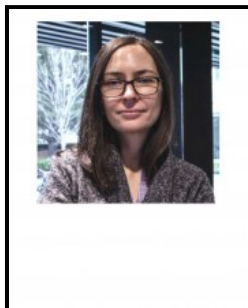




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LiNiO₂ as a high-entropy functional material**Kateryna Foyevtsova, University of British Columbia - Vancouver, Stewart Blusson
Quantum Matter Institute**

Research Associate

Virtual- SEE BIO Zoom
May 11, 2021 - 03:30 pm**Abstract:**

The 2015 discovery of entropy-stabilized transition-metal oxides, such as $\text{Mg}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Cu}_{0.2}\text{Zn}_{0.2}\text{O}$, [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 LiNiO_2 , 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 LiNiO_2 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 LiNiO_2 , as compared to similar cathode materials. The LiNiO_2 story showcases how insights from fundamental solidstate physics research can help advance technology.

[1] "LiNiO₂ 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).

[2] "Entropy-stabilized oxides", C. M. Rost et al., Nat. Commun. 6, 8485 (2015).

[3] "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:ZOOM <https://bit.ly/331Cik6>

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