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Hybrid functional studies of defects in layered transition metal oxides KHANG HOANG, North Dakota State University, MICHELLE JOHANNES, Naval Research Laboratory — Layered oxides $LiMO_2$ (M is a transition metal) have been studied extensively for Li-ion battery cathodes. It is known that defects have strong impact on the electrochemical performance. A detailed understanding of native point defects in $LiMO_2$ is however still lacking, thus hindering rational design of more complex materials for battery applications. In fact, first-principles defect calculations in $LiMO_2$ are quite challenging because standard density functional theory (DFT) calculations using the generalized gradient approximation (GGA) of the exchange-correlation functional fail to reproduce the correct physics. The GGA+U extension can produce reasonable results, but the transferability of U across the compounds is limited. In this talk, we present our DFT studies of defects in $LiMO_2$ (M=Co, Ni) using the Heyd-Scuseria-Ernzerhof (HSE) screened hybrid functional. The dominant point defects will be identified and compared with experiment; and their impact on the structural stability and the charge (electronic and ionic) and mass transport will be addressed. We will also discuss possible shortcomings of the HSE functional in the study of these electron-correlated materials.

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