

Unravelling polaron and bipolaron in (Li, Na)-doped V₂O₅ materials: DFT+*U* computational method

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Poster

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Pristine and (Li, Na)-doped (α , β)-V₂O₅ polymorphs emerging as quintessential exemplars in manifold of practical applications, especially for new generations of (Li, Na)-battery cathode materials, as well as for probing exotic fundamental electronic properties. α -V₂O₅ characterize as a d^0 charge-transfer insulator with strong O- p -V- d hybridization together with a large band gap, while β -Na_{0.33}V₂O₅ exhibits metal-insulator transition accompanied by a charge density wave (CDW) gap. With the highest oxidation state d^{+5} and layer structure, V₂O₅ has large potential to intercalate mobile alkaline (Li, Na) and alkaline earth elements which donate electrons to the framework. Consequently, the extra electrons routinely induce a polaronic mechanism in which they couple with available lattice distortions. It is a perennial issue that density functional theory (DFT) faces challenging to approach bandgap and strongly correlated properties. In this talk, we perform the rigorous Hubbard U correction (DFT+ U) to characterize exactly the band gap of d -state charge-transfer V₂O₅ insulator as well as the CDW gap of β -Na_{0.33}V₂O₅. Remarkably, our calculations showcase capacity to unravel the presence of the free polaron in Li-doped α -V₂O₅ as well as the coincident quantum criticality of bipolaron-to-polaron, and energetic favorable antiferromagnetic-to-ferromagnetic transitions in β -phase.

Keywords: V₂O₅, β -Na_{0.33}V₂O₅, charge-transfer insulator, polaron, bipolaron-to-polaron transition, ab initio method