

**Unravelling polaron and bipolaron in (Li, Na)-doped V<sub>2</sub>O<sub>5</sub> materials: DFT+U computational method****Huu T. Do***Department of Chemical Engineering, Chicago, Illinois, USA*Email: [huutdo09@gmail.com](mailto:huutdo09@gmail.com)**ID: PST02****Poster****Aug. 24, 16.00 - 17.30**

Pristine and (Li, Na)-doped ( $\alpha$ ,  $\beta$ )-V<sub>2</sub>O<sub>5</sub> 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.  $\alpha$ -V<sub>2</sub>O<sub>5</sub> characterize as a  $d^0$  charge-transfer insulator with strong O- $p$ -V- $d$  hybridization together with a large band gap, while  $\beta$ -Na<sub>0.33</sub>V<sub>2</sub>O<sub>5</sub> exhibits metal-insulator transition accompanied by a charge density wave (CDW) gap. With the highest oxidation state d<sup>+5</sup> and layer structure, V<sub>2</sub>O<sub>5</sub> 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 lonely 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 V<sub>2</sub>O<sub>5</sub> insulator as well as the CDW gap of  $\beta$ -Na<sub>0.33</sub>V<sub>2</sub>O<sub>5</sub>. Remarkably, our calculations showcase capacity to unravel the presence of the free polaron in Li-doped  $\alpha$ -V<sub>2</sub>O<sub>5</sub> as well as the coincident quantum criticality of bipolaron-to-polaron, and energetic favorable antiferromagnetic-to-ferromagnetic transitions in  $\beta$ -phase.

**Keywords:** V<sub>2</sub>O<sub>5</sub>,  
 $\beta$ -Na<sub>0.33</sub>V<sub>2</sub>O<sub>5</sub>,  
charge-transfer insulator,  
polaron,  
bipolaron-to-polaron  
transition, ab initio  
method