Passivation of Trap States in NiO

Scientific Achievement

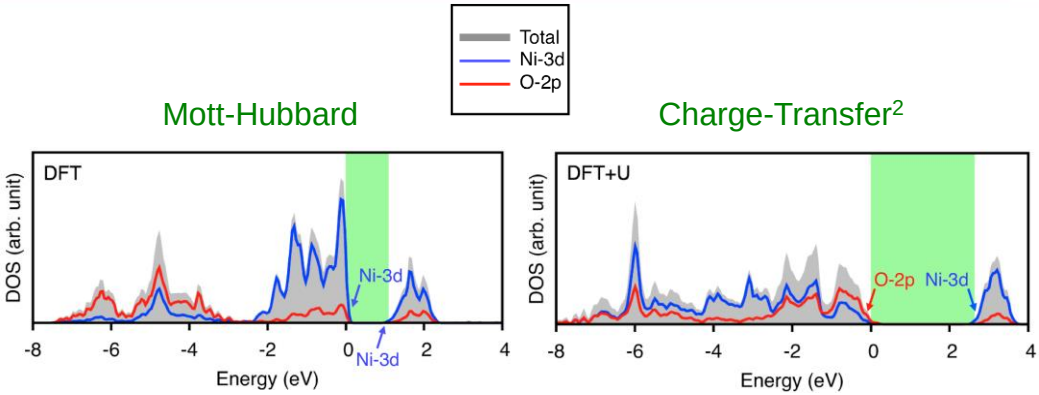
DFT+U calculation was used to understand how trap states are eliminated in the energy gap through passivating Ni-vacancy defects in NiO.

Significance and Impact

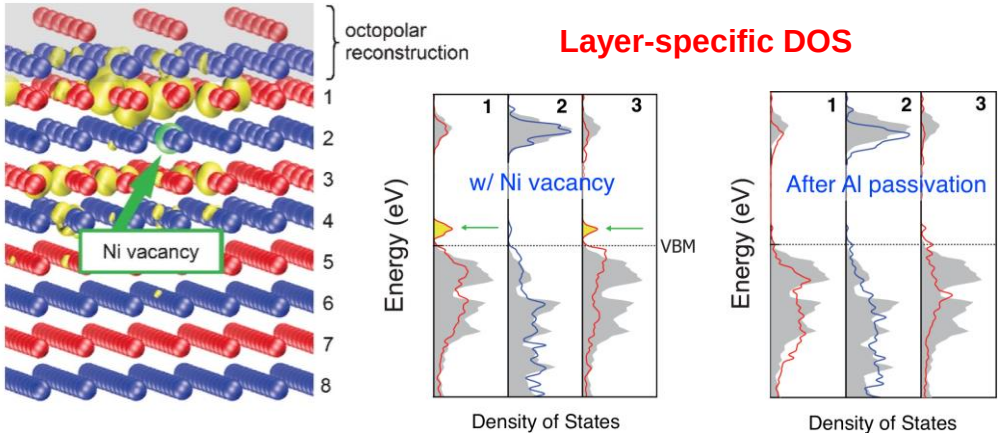
NiO is a promising p-type semiconductor for various solar-energy conversion technologies, but Ni vacancies are a major problem. Targeted Atomic Deposition (TAD) was developed to selectively passivate such localized defects, and first-principles calculation was used to provide a molecular level understanding of how trap states are eliminated.

Research Details

- **Localized trap states, which are deleterious to the performance of many solar energy materials, often originate from under-coordinated bonding associated with defects.**
- **Significant trap state density in NiO originates from under-coordinated oxygen atoms adjacent to Ni vacancies in the lattice.**
- **DFT+U correctly shows the Charge-Transfer energy gap in NiO as in the 1984 experiment[2] while DFT incorrectly shows the Mott-Hubbard behavior.**
- **Aluminum atoms, through the use of TAD, can effectively eliminate the localized trap states in the energy gap.**



1. Li, L.; Kanai, Y. Antiferromagnetic structures and electronic energy levels at reconstructed NiO(111) surfaces: A DFT + *U study*. *Phys. Rev. B* **2015**, *91* (23), 235304. http://dx.doi.org/10.1103/PhysRevB.91.235304
2. Sawatzky, G. A.; Allen, J. W. Magnitude and Origin of the Band Gap in NiO. *Phys. Rev. Lett.* **1984**, *53* (24), 2339-2342. http://dx.doi.org/10.1103/PhysRevLett.53.2339



Experiment–Theory Collaboration (Kanai, Cahoon) in UNC EFRC Photocathode Team

Work was performed at the University of North Carolina at Chapel Hill

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