Targeted Atomic Deposition for Defect Passivation

Scientific Achievement

Selective passivation of Ni vacancy defects in the widely used cathode NiO leads to dramatic optical and bleaching of thin films and to large improvements in the performance of dye-sensitized solar cells.

Significance and Impact

A new vapor-phase process termed Targeted Atomic Deposition (TAD) was used to passivate defects. The TAD process could be widely applied to defect passivation in semiconductor nanomaterials.

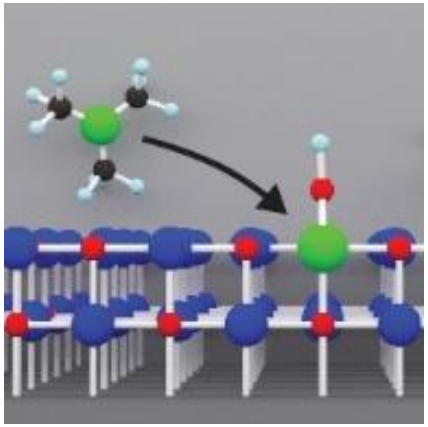
Research Details

- First-principles calculations identified oxygen-localized defect states as a result of Ni vacancies
- Vapor-phase trimethyl aluminum, at a temperature too low for layered deposition, selectively reacted with the oxygen dangling bonds at defect sites, removing trap states and bleaching thin films of NiO.

Flynn; McCullough; Oh; Li; Mercado; Farnum; Li; Donley; You; Nozik; McBride; Meyer; Kanai; Cahoon. ACS Appl. Mater. Interfaces **2016**, *8*, 4754-4761. DOI: 10.1021/acsami.6b01090

Localized vacancy defect states:

Vapor deposition at defect sites:



Untreated NiO: **TAD-treated:**

Work was performed at the University of North Carolina at Chapel Hill, the National Renewable Energy Laboratory, and Vanderbilt University.