Tuning the Electronic Levels of NiO with Alkali Halides

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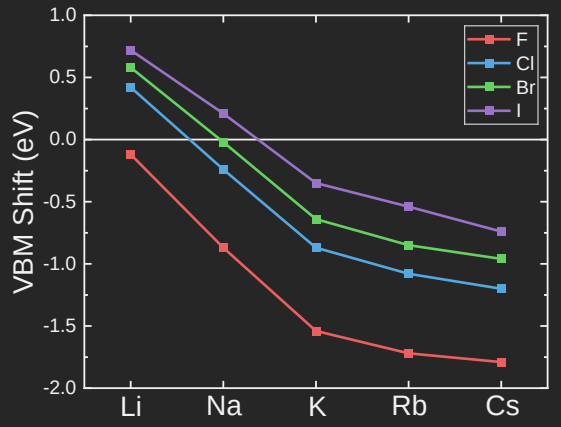
BACKGROUND: NiO is a very promising hole transport layer (HTL) for PSCs and being able to control its electronic levels in order to match those of the various perovskites is crucial. A surface modifier, such as the commonly used Alkali Halides (AX), could serve this purpose.

METHOD

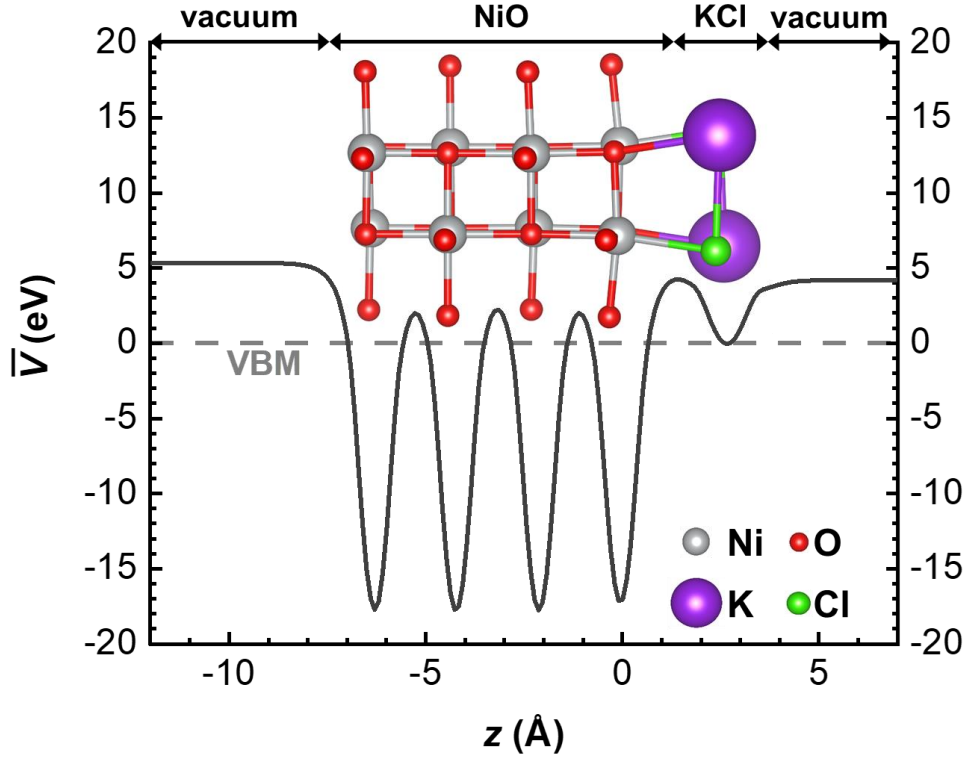
DFT calculations were performed in order to investigate how the adsorption of 20 different AXs affect the electronic levels of NiO.

RESULTS



1/8ML adsorption of different AXs on NiO surface can shift the valence band maximum (VBM) of NiO within a wide range of values.

Alkali Halides surface modifiers could **shift the electronic** levels of NiO for proper alignment with **any perovskite** for solar cell applications.

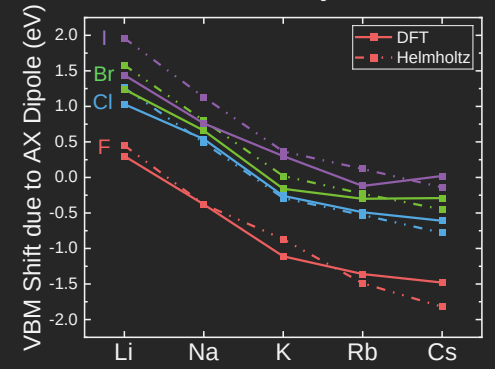


DIPOLE INDUCED SHIFT

Adsorbed AXs create an electric dipole on the surface of NiO, which is responsible for its VBM shift. Helmholtz Formula relates the VBM shift ΔV to the dipole moment change μ:

$$\Delta V = N\mu/\varepsilon_0$$

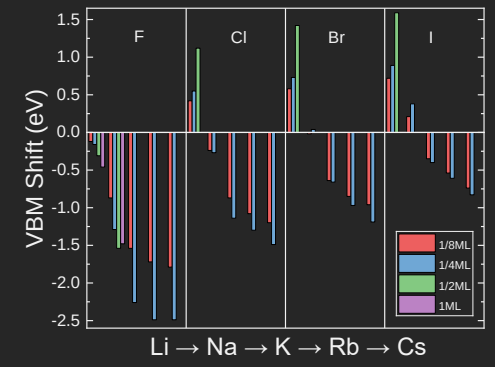
N: number of AX pairs per unit cell, ε_0: vacuum permittivity



The total shift is the sum of the dipole shift and a relatively constant shift due to charge transfer

INCREASED COVERAGE

This is not all! The VBM shift can become even larger, by increasing the AX coverage



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