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Title: First-Principles Calculation of Electronic Energy Level Alignment at Electrochemical Interfaces

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PII: S0169-4332(17)30812-7
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.03.147>
Reference: APSUSC 35523

To appear in: *APSUSC*

Received date: 11-2-2017
Revised date: 12-3-2017
Accepted date: 14-3-2017

Please cite this article as: Yavar T. Azar, Mahmoud Payami, First-Principles Calculation of Electronic Energy Level Alignment at Electrochemical Interfaces, *Applied Surface Science* (2017), <http://dx.doi.org/10.1016/j.apsusc.2017.03.147>

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- 1)-Using first-principles DFT calculation, we have determined the level shifts of the semiconductors TiO_2 and ZnO at the interfaces with MeCN and DMF solvent molecules.
- 2)-The level shifts of semiconductor is obtained using the potential difference between the clean and exposed surfaces of asymmetric slabs.
- 3)-It is shown that the solvent molecules give an up-shift to the levels, and the amount of this shift varies with coverage.
- 4)-Molecular dynamics simulations of the interface have shown that at room temperatures the semiconductor surface is not fully covered by the solvent molecules.

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