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

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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.