Computational Study of Conduction and Breakdown Mechanisms in Metal Oxide Dielectric Insulators

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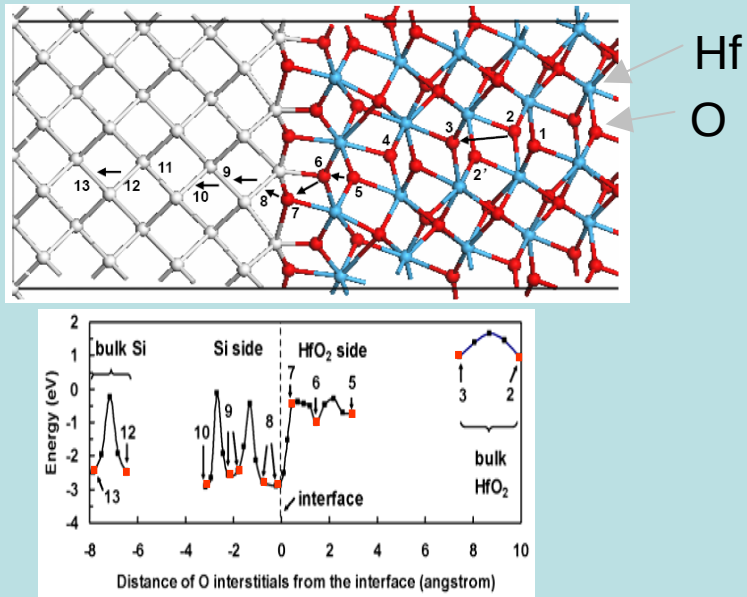
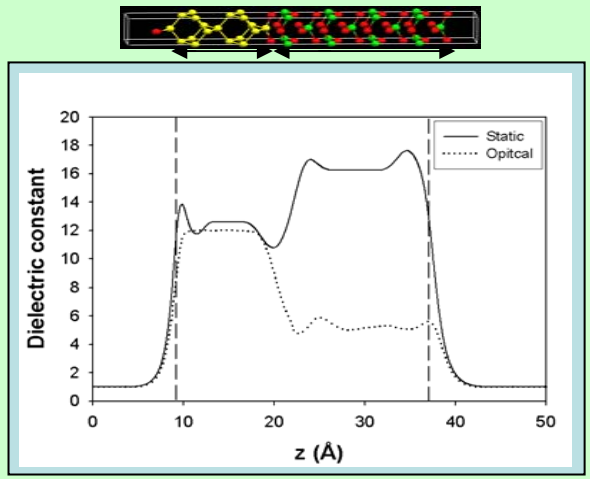
Density functional theory calculations to determine ***point defect dynamics*** & ***position dependent dielectric constant and band structure profiles of*** **Si-HfO_2 interfaces**

O Interstitial Dynamics



Dielectric Constant Profile



Band Structure Profile