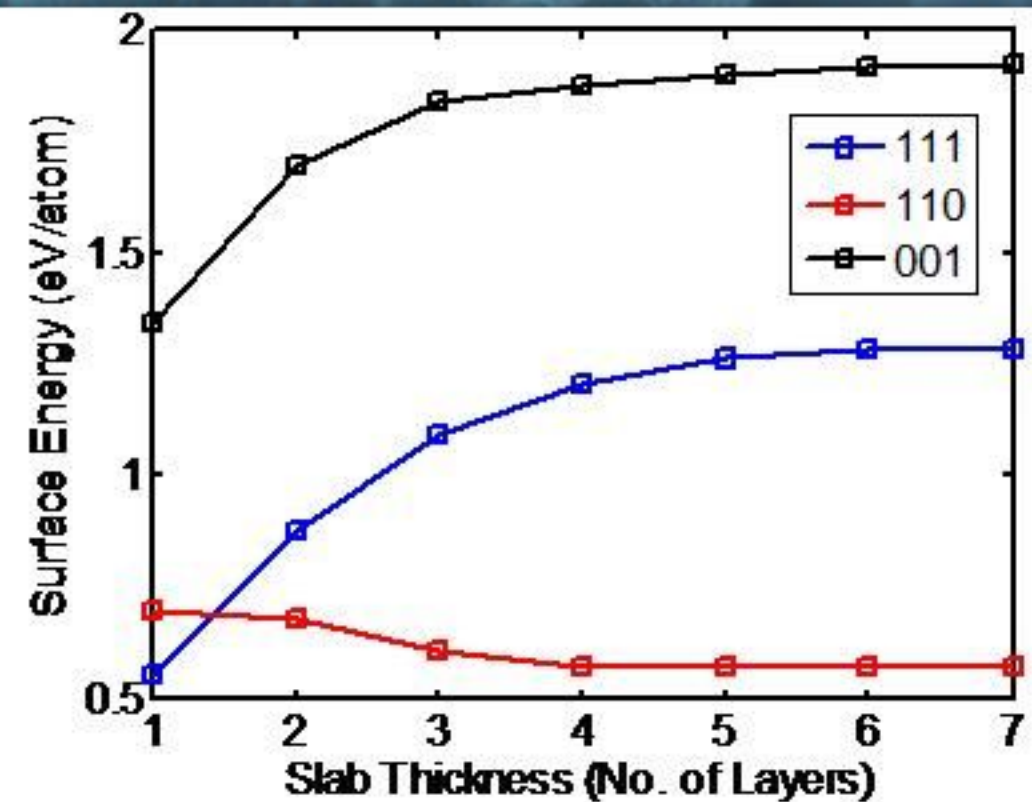


• Initial Investigation

- » First principles based study
 - ✓ Surface energetics of clean, unreconstructed surfaces.
 - ✓ Initial chemisorption pathway of ALD based oxide deposition.
 - ✓ Surface dependent defect formation energies.
 - ✓ Composite D.O.S.

• Initial results (GaAs)

- » (110) clean surface most stable energetically.
- » H passivation unfavorable, OH passivation favorable energetically
- » (111)B adsorbs $\text{Al}(\text{CH}_3)_3$ 'better' than (111)A – cue Self Cleaning effect?



Initial chemisorption energies GaAs and Si

