Dielectric charging: First-principles study of defects in a-Si_3N_4 and a-SiO_2

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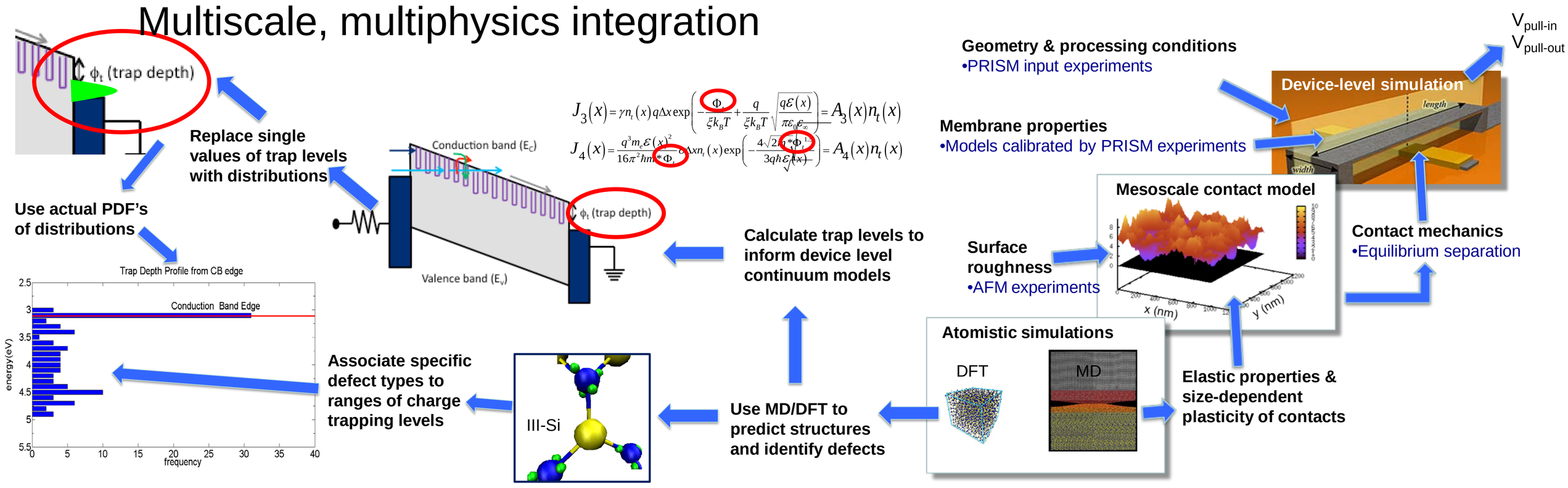
Introduction and Motivation

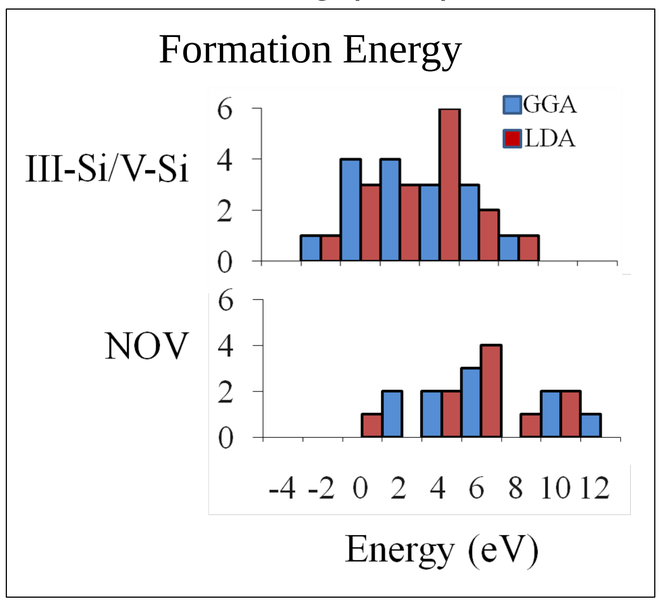
- Dielectric charging is one of the most prominent modes of degradation and device failure in the PRISM RF-MEMS device
- Charging is the result of negative charge build-up from electron capture by point defects

Multiscale, multiphysics integration

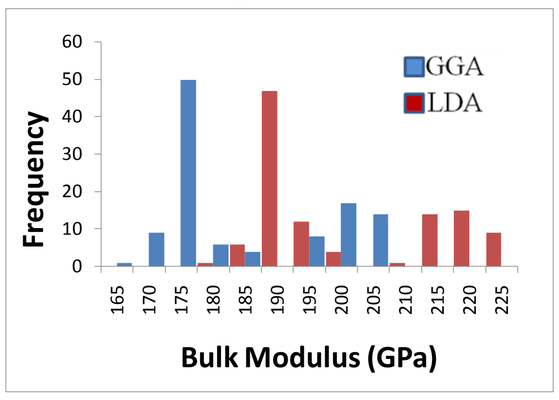


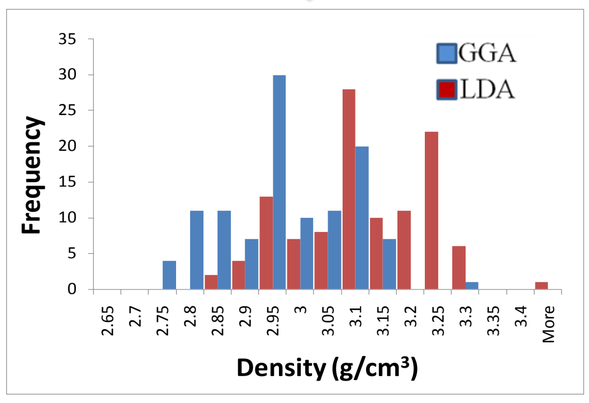
Two Sources of Uncertainty: Intrinsic Atomic Variability and Model Form

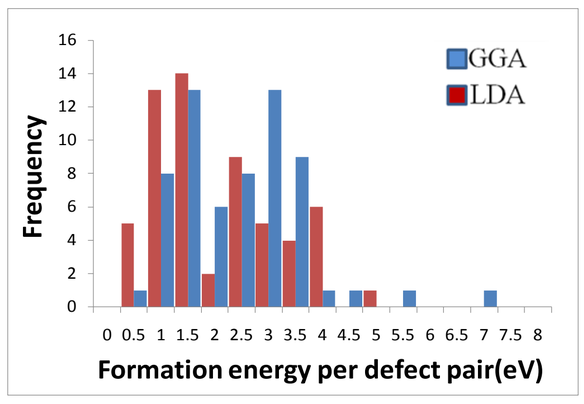
- Amorphous materials have no long range order and variability in medium range order
- Proper correction of charge divergence in amorphous periodic systems (LMCC) is atomic location dependent
- DFT calculations involve self-consistently solving the Kohn-Sham equations: $\left[\frac{1}{2}\nabla^2 + v_{eff}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r}) \quad ; \quad n(\mathbf{r}) = \sum_{i=1}^{N}|\psi_i(\mathbf{r})|^2$
- v_{eff} term in these equations contains an approximated exchange-correlation functional
- Overbinding (LDA) and underbinding (GGA) extremes calculated to provide model form estimate



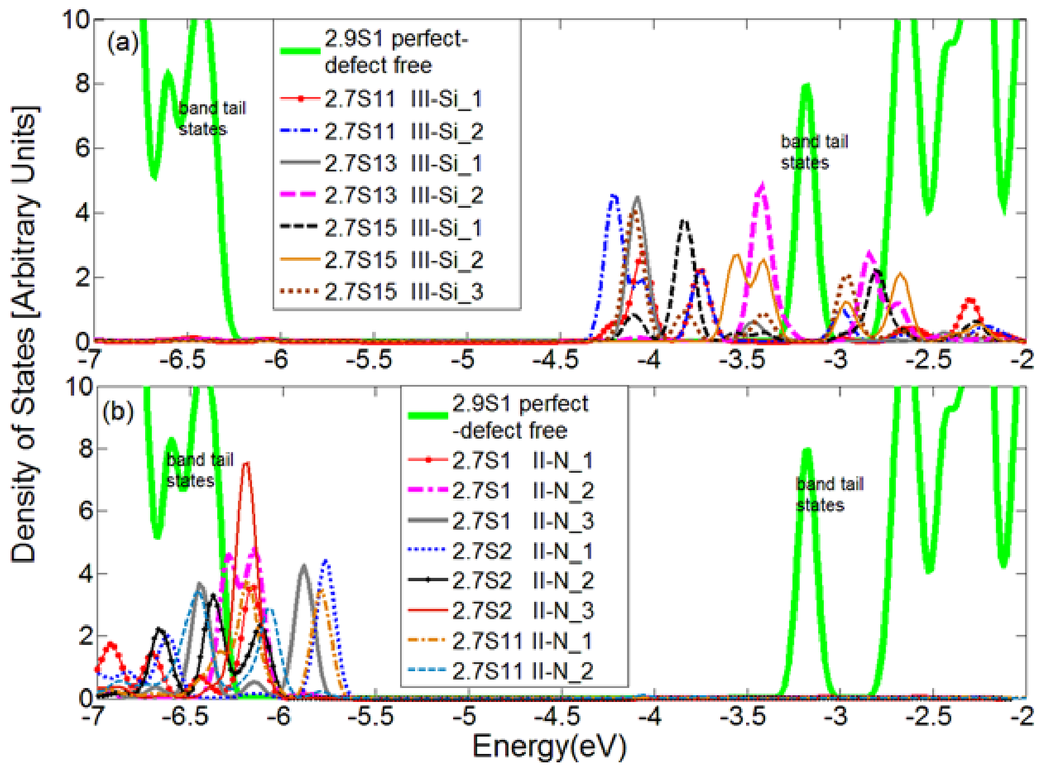
Distributions of properties for each functional show intrinsic variability is at least 3X greater than model form !!!

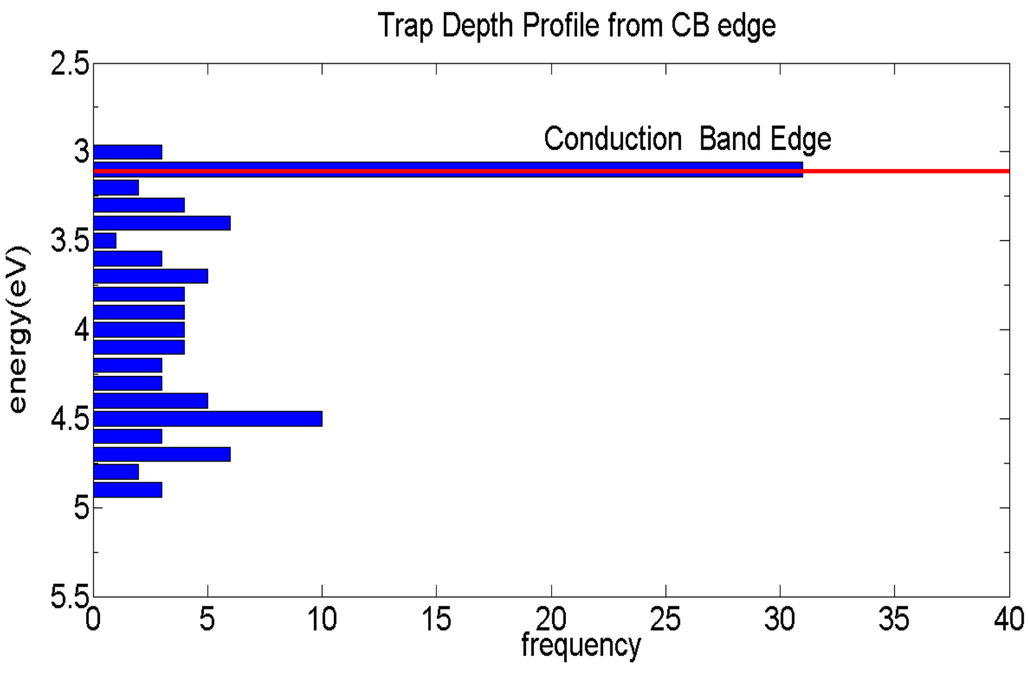






Density of States and Charge Transition Levels





Defects have a distribution of associated properties (e.g. formation energies and electronic energy levels).

Conclusion

- Ensemble of structures capture atomic variability inherent in amorphous materials
- Single trap depth value is replaced by probability distribution that covers a range of values in dielectric charging models
- Empiricism of continuum charging model reduced and predictive power is expanded across spatial and temporal scales
- Intrinsic variability of amorphous atomic network is on average a factor of four greater than model form uncertainty

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Ref: [1] N.L. Anderson *et al.*, Phys. Rev. Lett. 106, 206402 (2011)
[2] R.P. Vedula *et al.*, submitted to PRB (in review).
[3] N.L. Anderson *et al.*, in preparation for PRL.
[4] R.P. Vedula *et al.*, in preparation for PRL.