PROJECT OVERVIEW: Atomistic Modeling of Metallic Conduction Limits in Quasi 1-D Silicon Nanowires

I INTRODUCTION

- Experiments observed tunability between metallic and insulating behavior in ultra-thin, highly-doped Si:P nanowires
- Charge carrier localization induced by random doping fluctuations likely cause of metallic conduction limits

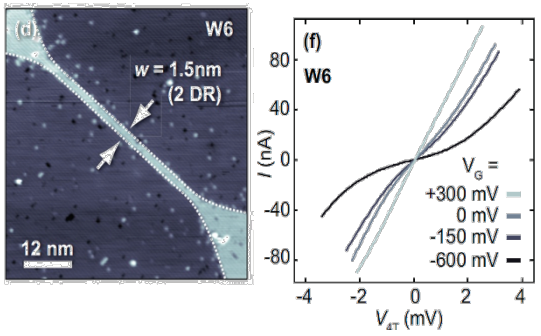
II METHODOLOGY

- Large-scale atomistic modeling (NEMO)
- Self-consistent TB simulations of bandstructure / density of states (DOS)

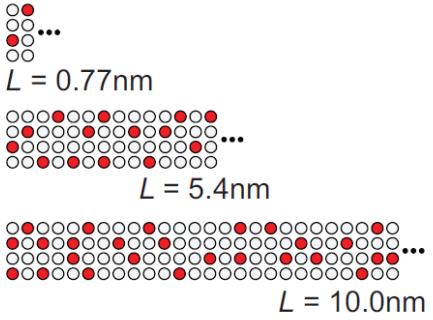
III RESULTS

- Successfully modeled disordered nanowires up to 10nm in length
- Observation of DOS energy gap for 10nm wire shows trend towards carrier localization
- Published in *PRL* 113, 246802, 2014, B. Weber, H. Ryu, Y.-H. M. Tan, et.al.

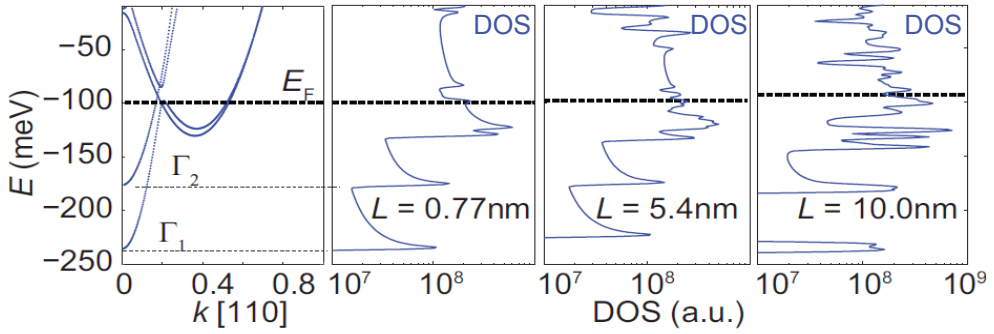
1 STM plot / IV-curve of nanowire



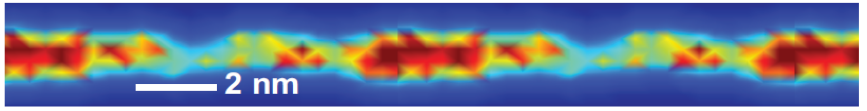
2 Atomistic doping profiles



3 Bandstructure / DOS of nanowire, L= 0.77nm, 5.4nm, 10nm



4 Charge density 10nm wire (repeated supercells)



1) STM image of Si:P nanowire, I-V curve shows non-linear behavior for negative gate biases **2)** Doping profiles for NEMO calculation **3)** Calculated DOS of different disordered wires **4)** 10nm long, disordered wire shows charge carrier localization