

PROJECT OVERVIEW: Empirical / Atomistic Modeling of Binding Energies in Phosphorus Donor Clusters

I INTRODUCTION

- Si:P Double Quantum Dot (DQD) device
- What is the number of P dopants in clusters D_1 and D_2 ?

II METHODOLOGY

- Atomistic modeling of binding energies with NEMO3D-peta
- Empirical modeling of millions of donor cluster configurations

III RESULTS

- Accurate determination of P dopants in clusters D_1 and D_2 using binding energy confidence bands
- Development of empirical models for rapid calculation of donor cluster binding energies
- Published in *Nature Nanotechnology*, 9, 430, 2014 (B. Weber, Y.-H. M. Tan, et.al.)
- Manuscript in preparation (Tan, et.al.)

