TOWARD QUANTITATIVE PREDICTION OF DEFECT TOLERANCE IN SEMICONDUCTORS: LEVERAGING HPC AND PHYSICAL INSIGHTS TO DESIGN RADICALLY CHEAPER ENERGY MATERIALS

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EXECUTIVE SUMMARY

Climate change is a critical challenge confronting this generation, and if we are to address it, part of the solution must include a decarbonized electricity sector. Photovoltaic (PV) solar cells will undoubtedly play a vital role in this transition. My research aims to discover new materials that have a high potential to drastically lower the cost of PV solar cells. Performance of these new materials is less sensitive to imperfections in their atomic structure, permitting the use of simpler methods for their manufacturing, such as solution processing. We approach this problem through quantum mechanical calculations of the atomic-scale physics of the defects themselves to build a detailed understanding of what makes defects detrimental in materials such as silicon—the dominant PV material today—and relatively benign in others. This will eventually enable the design of defect-tolerant materials for the next generation of PV technologies.

RESEARCH CHALLENGE

My work aims to understand the Ångstrom-scale physical mechanisms underlying defect-tolerant behavior in some semiconductors. Materials such as silicon—the active material in approximately 90% of the PV market today—require an extremely high degree of purity and crystalline perfection in order to perform well, while some newly discovered materials can achieve high efficiencies despite the presence of many defects. However, all such materials prompt concerns surrounding elemental scarcity, toxicity, and stability. Understanding the physics behind the defect-tolerant behavior would enable us to engineer similar materials that do not suffer from these drawbacks and could potentially revolutionize the PV industry and more effectively combat climate change.

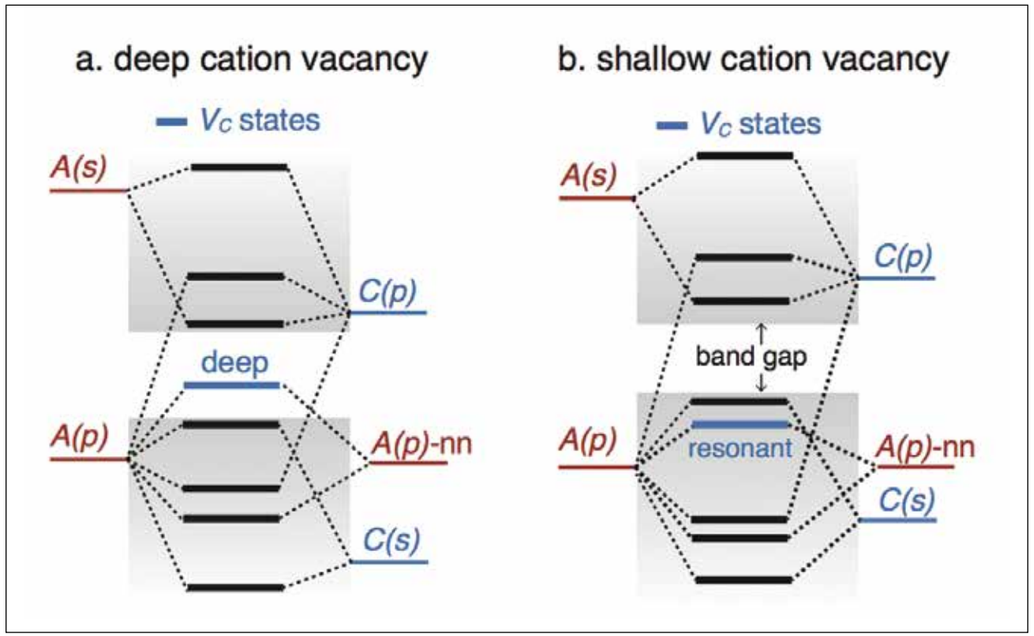

Figure 1: This figure shows molecular–orbital-type band structures of ns^2 compounds featuring deep (a) and shallow (b) cation vacancies. A key finding of our work was the importance of aligning the orbital energies of the anion-*p* and cation-*s* states to enable larger band dispersion and hence shallow cation vacancy states.

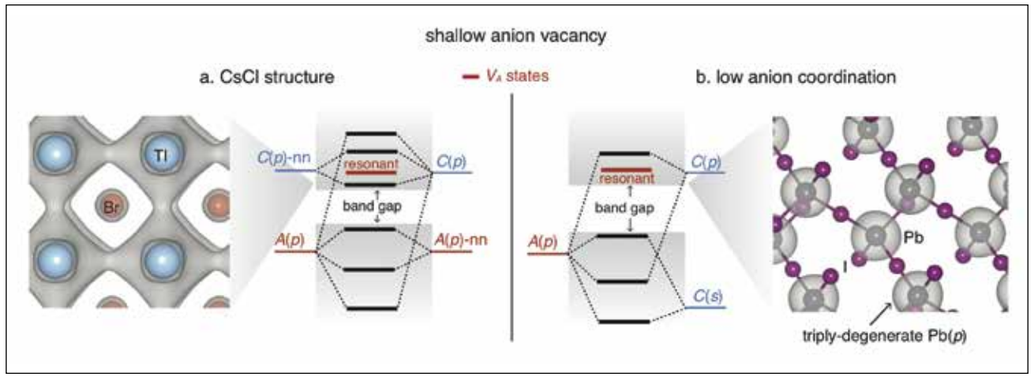

Figure 2: This figure, in turn, shows strategies for realizing shallow anion vacancies, which are related to crystal structure rather than chemistry. Part (a) shows a symmetry-enforced ionic structure, while (b) illustrates low anion coordination.

METHODS & CODES

We seek to understand the physics of crystalline defects through quantum mechanical calculations performed within the density functional theory formalism as implemented in the VASP code. We computed formation energies and charge transition levels of various defects of interest in order to understand trends in this behavior across a wide array of compounds.

RESULTS & IMPACT

The key impact of this work would be a drastic improvement in the ability of computer simulations to inform and guide materials design and discovery—the tasks that, at the moment, are mostly done by trial and error or intuition. Our work is part of a coming revolution in HPC-aided precision materials design that is capable of targeting specific properties and functionalities of interest to science as well as society.

WHY BLUE WATERS

The funding from the Blue Waters graduate fellowship, the community of fellows and of NCSA staff, more broadly, was key to my intellectual independence as well as my becoming a member of the HPC community.

PUBLICATIONS & DATA SETS

Kurchin, R.C., et al., Structural and Chemical Features Giving Rise to Defect Tolerance of Binary Semiconductors. *Chemistry of Materials*, 30:16 (2018), pp. 5583–5592.

Rachel Kurchin is a fourth-year PhD student in materials science and engineering at the Massachusetts Institute of Technology. She works with Tonio Buonassisi and expects to graduate in December 2019.