Molecular dynamics and many-body perturbation theory analysis of defects in monolayer germanium monochalcogenides

Defects can strongly influence the electronic properties of semiconducting materials, particularly in 2D or quasi-2D configurations, because of the reduced screening environment. Here, we study the structural and optoelectronic properties of defects within monolayer germanium monochalcogenides. Using reactive molecular dynamics to simulate various mechanisms for defect formation, we identify characteristic defects that occur within the monolayer. Additionally, we apply first-principles many-body perturbation theory within the GW/BSE approximation to investigate the influence of selected defects on the optoelectronic properties of the materials. We determine that the optoelectronic properties are significantly influenced by the presence of these defects.

The authors acknowledge funding support from the Department of Energy (Award #DE-SC0018080) and computational resources from DOE NERSC, MGHPCC and NSF-XSEDE.

* The research work was carried out under the grant of National Science Foundation (NSF), DMR-1610031.
* We acknowledge the Boston University Scientific Computing Center for computational resources.

This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562. Specifically, some calculations were performed on Stampede2 at TACC through allocation TG-DMR160012.

Additional computational resources were provided by the Boston University Shared Computing Cluster (SCC) at the Massachusetts Green High Performance Computing Center (MGHPCC).

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Two-dimensional (2D) or quasi-2D materials show great promise for optoelectronic and photonic applications, particularly because of the ability to tune bandgaps and other properties via strain, doping and layering of different materials.1–3

Defects in semiconducting materials can introduce localized states in the electronic bandstructure, resulting in bound excitons.

The reduced screening environment and tighter localization of electronic wavefunctions in low-D materials tend to magnify the effects of defects.4

Defect-bound excitons typically have stronger electron-hole binding and electron-phonon interactions as well as longer lifetimes.

The presence of defects can therefore be harmful to the optoelectronic function of materials, but may also be harnessed for applications such as single-photon emitters and catalysis.5

**Defect Geometry with ab initio Molecular Dynamics**

Calculates forces on nuclei at each timestep as a function of ground state electronic Hamiltonian

No empirical parameters

Allows simulation of defect formation through heating, ion bombardment, etc.

Allows comparison of stability of different 2D structures

**Excited States with Many-body perturbation theory (MBPT)**

Electrons and excitons treated as “quasi-particles”: particle plus the disturbance it causes

ASK SAHAR about including mention of reactive force field MD, and about Kirk printing on Saturday morning (and having to pay ~$100)

Make an “Action-y” image of MD on the supercell

Double-check availability of printer on Friday (latest availability)

The thing about different allotropes6

Kirk Stuff7,8

**Optoelectronic Properties**

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