

Formation and Migration of Vacancy Defects in Silicon Carbide

Elizabeth M. Y. Lee[†], Giulia Galli^{†,‡}, and Juan J. de Pablo^{†,‡}

[†]Pritzker School of Molecular Engineering, The University of Chicago, Chicago, IL, USA

[‡]Material Science Division, Argonne National Lab, Argonne, IL, USA



Introduction

Spin defects in diamond and silicon carbide (SiC) are promising platforms for quantum information science applications. SiC is a particularly attractive material because of its ease of growth and microfabrication compared to diamond, and its integrability into existing optoelectronic devices. Divacancy defects in SiC have been shown [1,2] to host optically active electronic spins with long coherence times even at room temperature, thus providing a basis for quantum technologies. However, the formation mechanism and migration properties of point defects in SiC are poorly understood and hence difficult to control.

Using advanced simulation techniques, we gain insight into the creation, interaction and migration of vacancies in SiC, aimed at deriving rules for the design of robust defects in scalable quantum materials. In particular, we used a combination of enhanced sampling methods [2] coupled with classical Molecular Dynamics to investigate mechanisms of the formation and migration of vacancy defects in 3C-SiC.

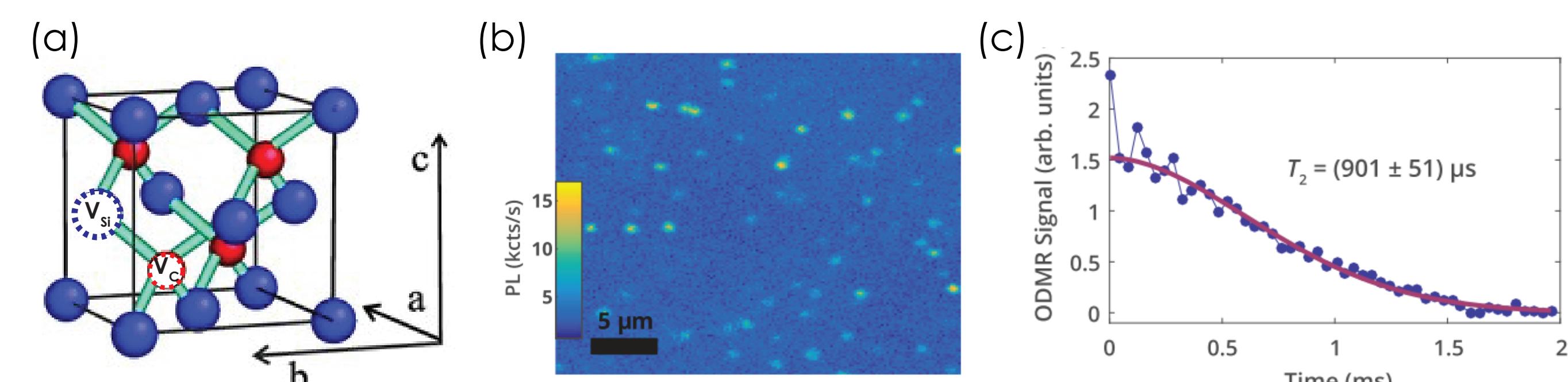


Figure 1: Divacancy of 3C-SiC. (a) The crystal structure of 3C-SiC with a divacancy, $V_{\text{Si}}V_{\text{C}}$. (b) A two-dimensional photoluminescence scan showing single defects as isolated luminescent spots in 3C-SiC. (c) Hahn-echo measurement performed on an ensemble of neutral divacancy defects in the higher-irradiation 3C-SiC sample ($1 \times 10^{15} \text{ cm}^{-2}$ fluence) at $T = 20 \text{ K}$ and $B = 253 \text{ G}$, showing $T_2 = (901 \pm 51) \mu\text{s}$. Panels (b) and (c) are adapted from Ref. [2].

Atomistic Simulation of SiC

We simulate defects in SiC via an all-atom classical Molecular Dynamics (MD) using a 3-body semiempirical potential known as EDIP [3] as implemented within LAMMPS software suite. We performed NPT and NVT simulations at 1 atm using Nose-Hoover barostat and thermostat.

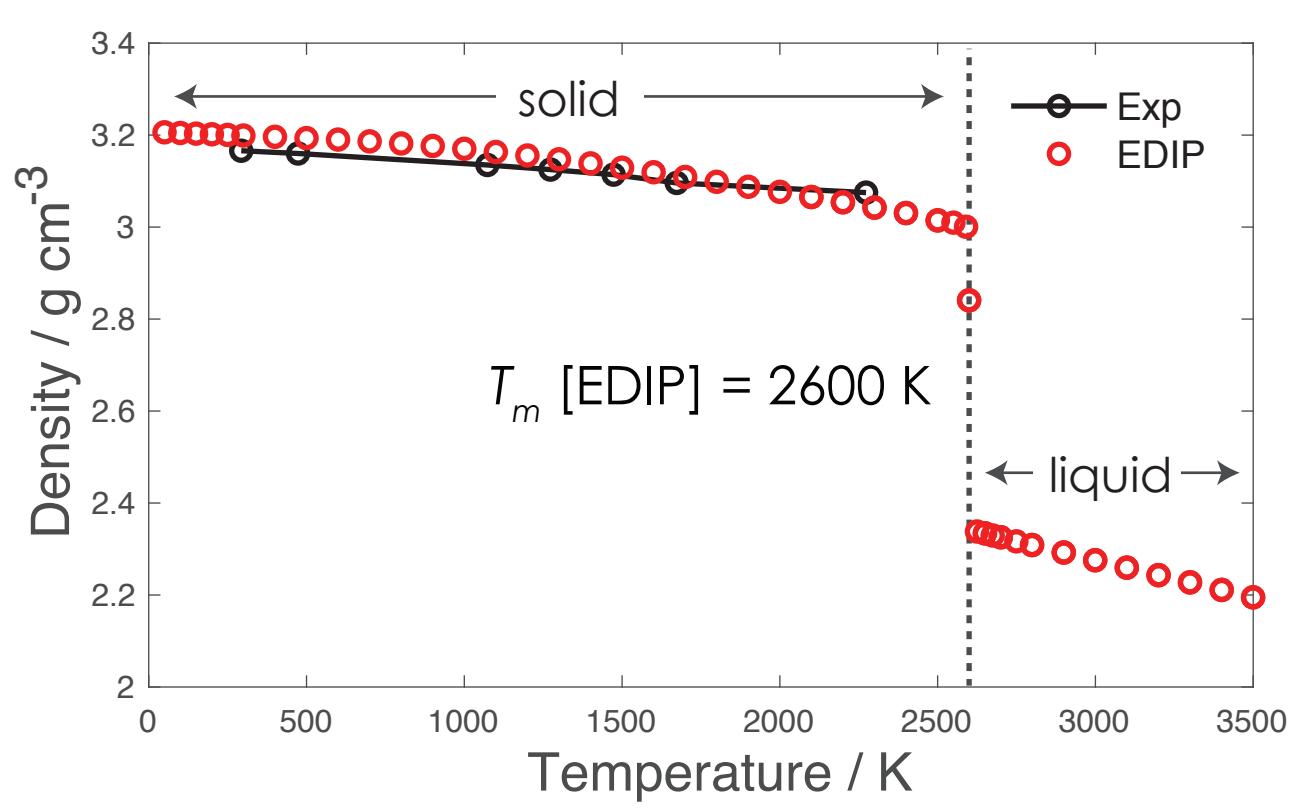


Figure 2: Temperature-dependent density of the bulk solid predicted using the EDIP potential is in a good agreement with experiment [4] within the range of typical annealing temperature (1100 - 2100 K). The predicted melting point of bulk 3C-SiC from MD simulations is 2600 K, which slightly underestimates the experimental value of 2730 K.

Voronoi-based Defect Analysis

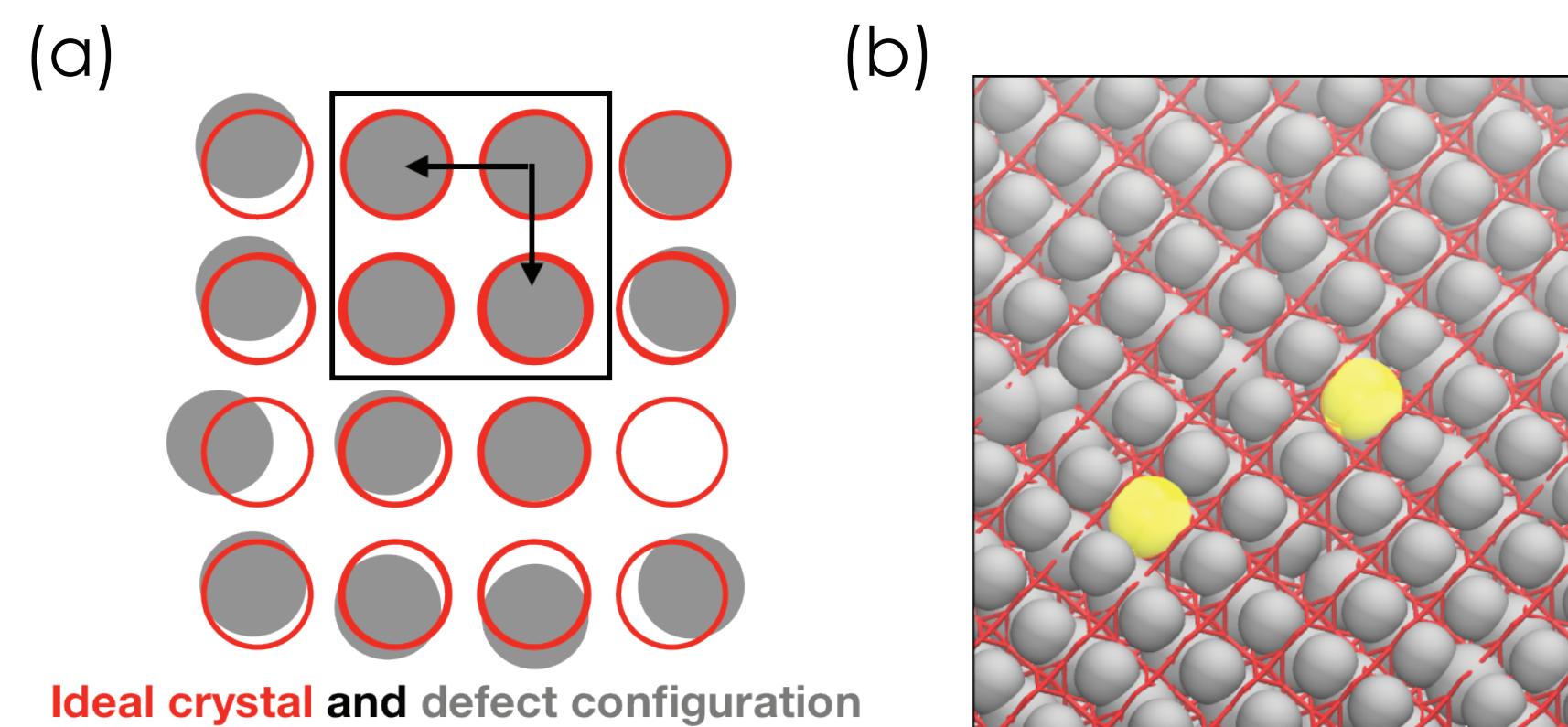


Figure 3: Vacancy Identification. (a) Construction of a reference (crystalline) configuration based on the MD snapshot. (b) Vacancies (in yellow) and the associated voronoi tessellation of the reference configuration (red lines)

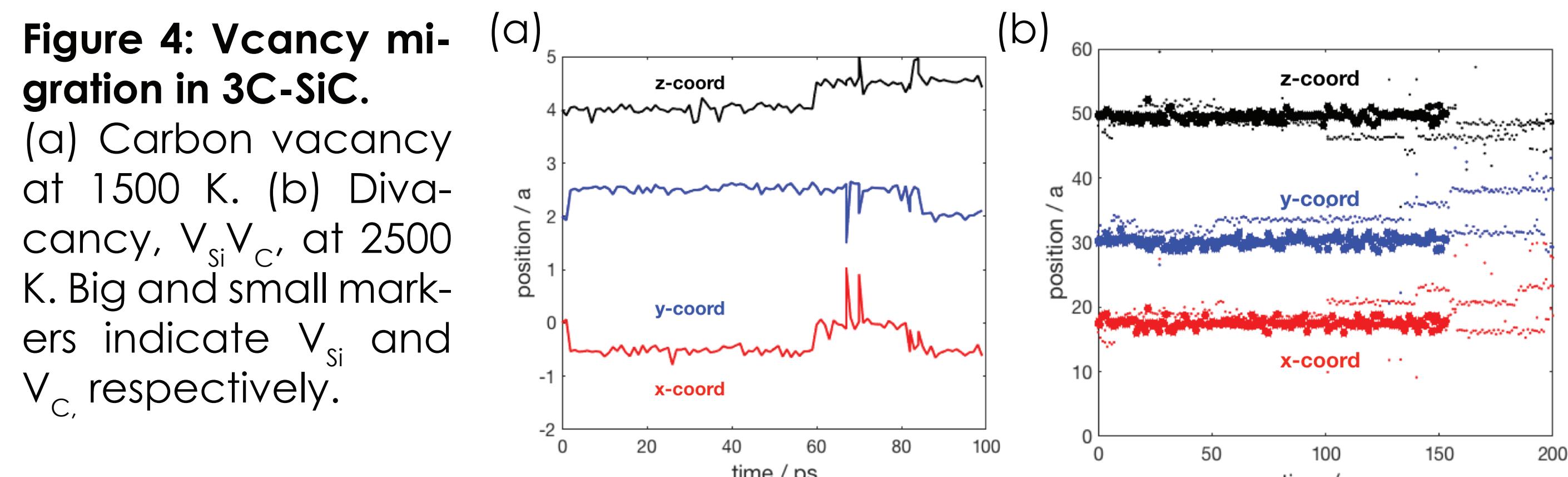


Figure 4: Vacancy migration in 3C-SiC. (a) Carbon vacancy at 1500 K. (b) Divacancy, $V_{\text{Si}}V_{\text{C}}$, at 2500 K. Big and small markers indicate V_{Si} and V_{C} , respectively.

Mapping the Free Energy Landscape of Vacancy Migration

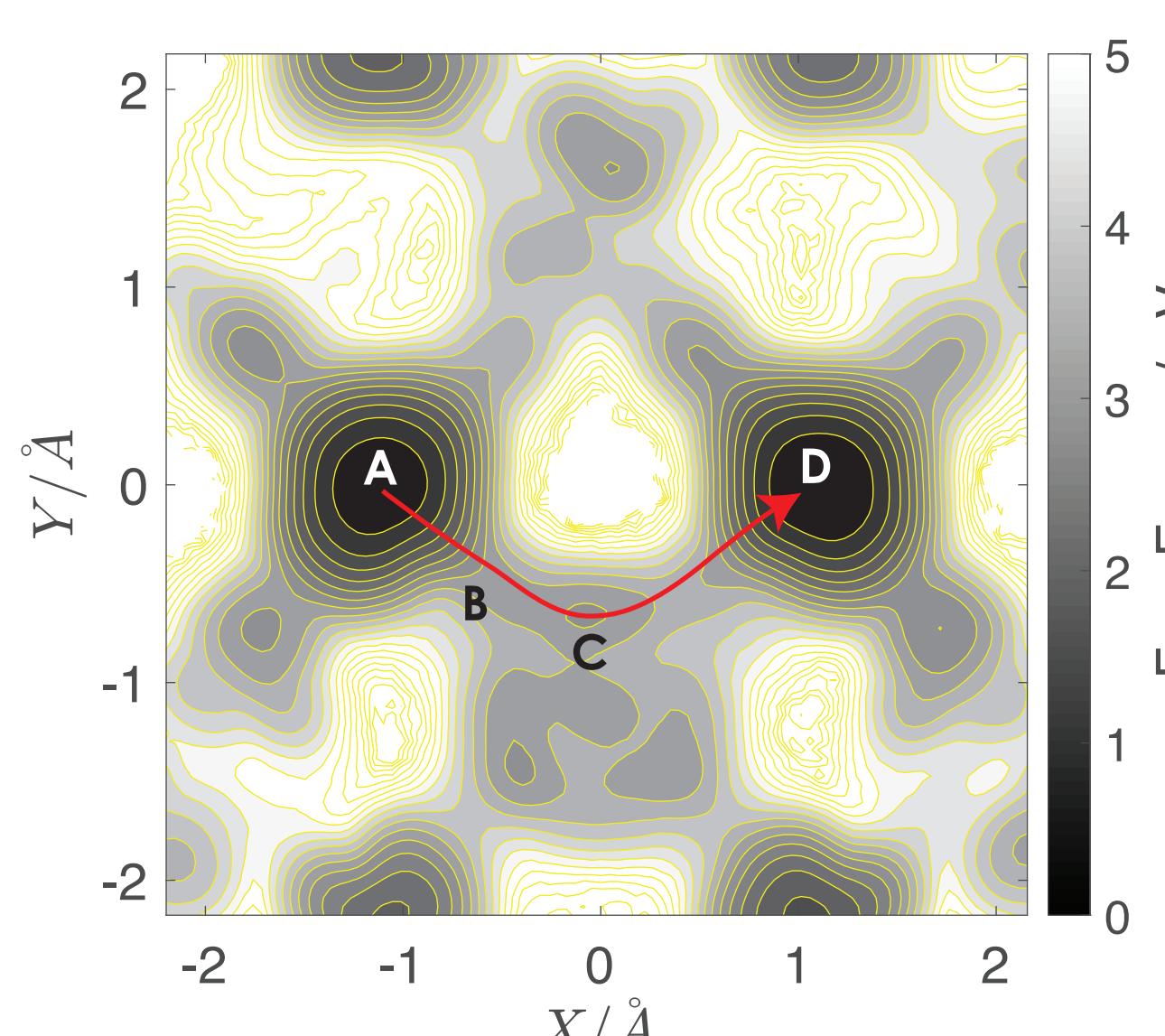
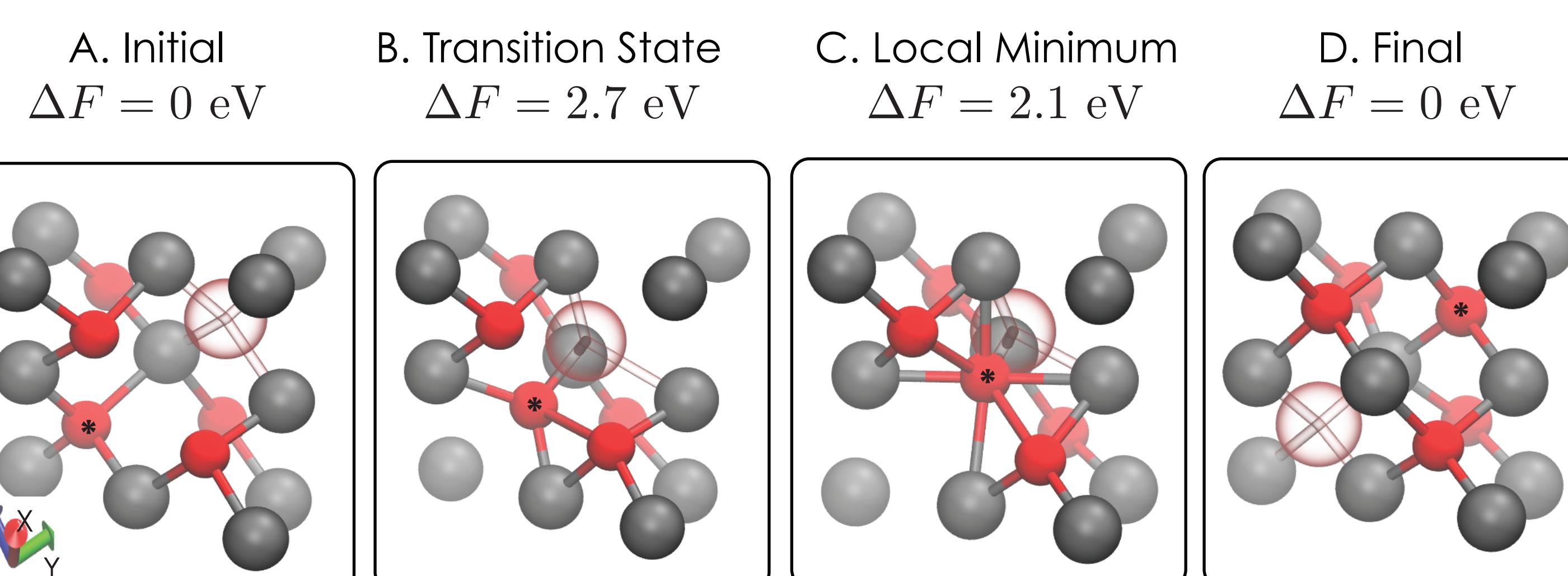
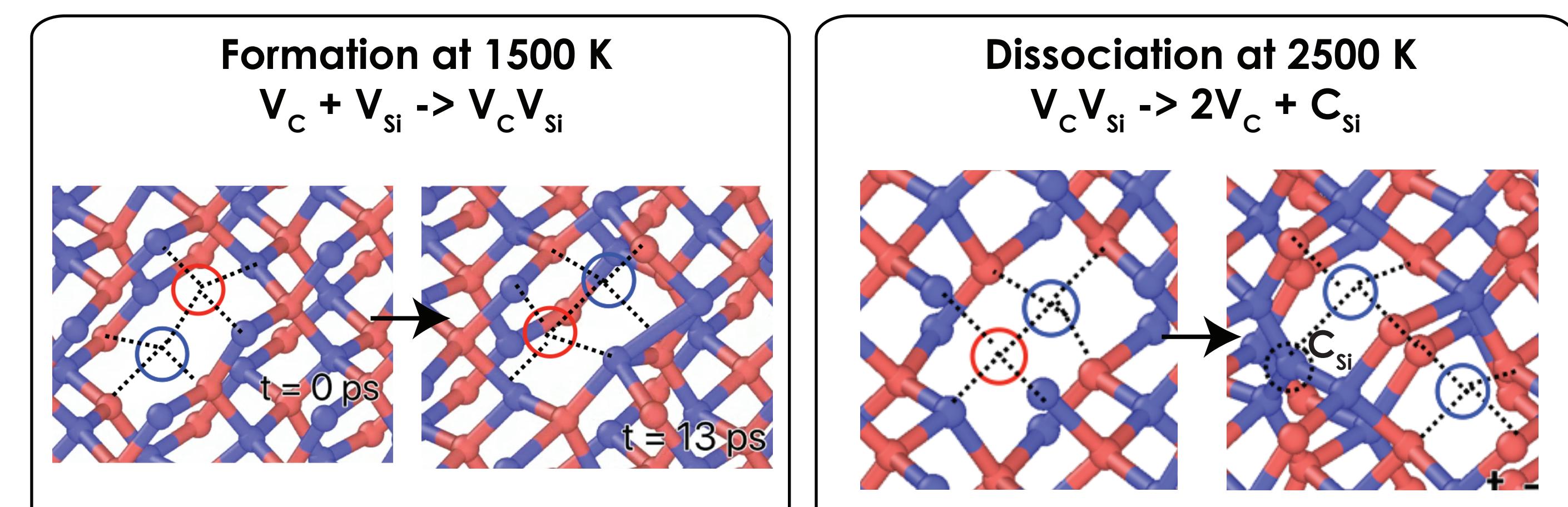


Figure 5: Free energy map of a carbon vacancy migration in 3C-SiC at 1500 K. X and Y coordinates are the relative cartesian coordinates with respect to the carbon atom displacing the vacancy. Red arrow indicates the transition path from the initial and final states with the following labels for each state: initial (A), transition state (B), local minimum (C), final



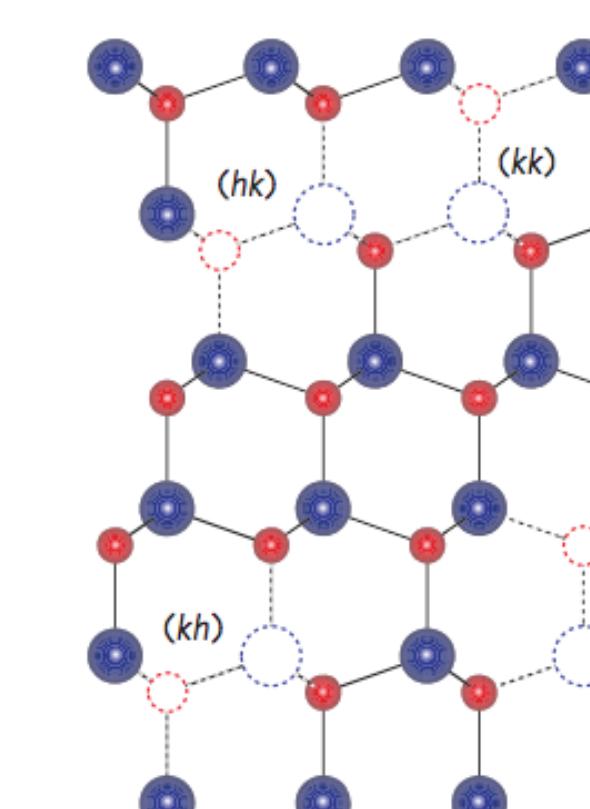
Gray and red spheres represent silicon and carbon atoms, respectively. Carbon vacancy atom is indicated by a semi-transparent red sphere, which exchanges its position with a neighboring carbon atom (marked by *).

Temperature-Driven Formation and Dissociation of Divacancies



Red and blue spheres represent silicon and carbon atoms, respectively. Silicon and carbon vacancies are indicated by red and blue open circles.

Future Directions



We plan to map out the free energy landscape of divacancy formation and dissociation as seen in unbiased MD simulations to identify pathways leading to creation and annihilation of divacancy complexes. Electronic structure calculations using Density Function Theory will be applied to obtain electronic properties of defects along the identified transition pathways. We will extend our method to study vacancy defects in 4H-SiC (left figure) and in other quantum materials.

References

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Acknowledgments

We thank Chicago Research Computing Center and the Laboratory and Computing Resource Center at Argonne National Laboratory for providing computational resources to enable this work. This project is funded by the Midwest Integrated Center for Computational Materials (MICCoM) as part of the Computational Materials Sciences Program funded by DOE/BES.

