

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Dynamics of vacancies in two-dimensional Lennard-Jones crystals**<sup>1</sup> ZHENWEI YAO, MONICA OLVERA DE LA CRUZ, Northwestern University — Vacancies represent an important class of crystallographic defects, and their behaviors can be strongly coupled with relevant material properties. We report the rich dynamics of vacancies in two-dimensional Lennard-Jones crystals in several thermodynamic states. Specifically, we numerically observe significantly faster diffusion of the 2-point vacancy with two missing particles in comparison with other types of vacancies; it opens the possibility of doping 2-point vacancies into atomic materials to enhance atomic migration. In addition, the resulting dislocations in the healing of a long vacancy suggest the intimate connection between vacancies and topological defects that may provide an extra dimension in the engineering of defects in extensive crystalline materials for desired properties.

<sup>1</sup>We thank the financial support from the U.S. Department of Commerce, National Institute of Standards and Technology, the Office of the Director of Defense Research and Engineering (DDR&E) and the Air Force Office of Scientific Research.

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Date submitted: 07 Nov 2014

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