B MÔN TIN V T LÝ, KHOA V T LÝ, TR NG Đ I H C KHOA H C T NHIÊN HÀ N I

Department of Computational Physics and Applied Informatics respectfully invites you to our monthly Seminar sponsored by Faculty of Physics

Seminar

Date: Fri. 24th June / Time: 9 am – 11 am / Place: Room 408F, Building T1

334 Nguy n Trãi, Thanh Xuân, Hà N i

Kính m i m i ng i đ n d / Everyone is welcome !

(Keynote) Speaker 1 (9 am - 10 am):

Dr. Le The Anh (School of Materials Science, Japan Advanced Institute of Science and Technology)

Title: ***First-principles study of hydrogen-enhanced phosphorus diffusion in silicon***

Abstract: In recent years, impurity doping in silicon by the catalytic-chemical vapor deposition method has gained technological importance because of the capability of low-temperature and large-area doping. In this method, mono-atomic H is incorporated in silicon along with impurity

atoms as a result of decomposition of hydrides of source materials. This suggests H-enhanced diffusion of phosphorus (P) that is the most widely used donor in Si [1-3]. In this study, we present a first-principles study on the interstitial-mediated diffusion process of neutral P atoms in a Si crystal with the presence of H. By relaxing initial Si structures containing a P atom and an H atom, we derived four low-energy P-H-Si defect complexes whose formation energies are significantly lower than those of P-Si complexes. We found that the H atom pairs with either P or Si atom and changes the nature bonding between P and Si atoms from out-of-phase conjugation to in-phase conjugation. This fact results in the lower formation energies compare to the cases without H atom. For the migration, we have found that P-H-Si complexes can migrate with low barrier energies if an H atom sticks to either P or Si atom. Energy barriers for the migration of a neutral P atom in Si without an H atom, ranging from 0.1 to 0.7eV [4, 5], are comparable to that of the migration of P-H-Si complexes. The low activation energy in the present case, therefore, is attributed to low formation energies of P-H-Si complexes in comparison to those of P-Si complexes. ***Details of the study are published in*** **the J. of Appl. Phys. 119, 045703 (2016).**

[1] Appl. Phys. Lett. **63**, 3060 (1993).

[2] Jpn. J. Appl. Phys. **34**, L1325 (1995).

[3] Jpn. J. Appl. Phys. **50**, 121301 (2011).

[4] Appl. Phys. Lett. **82**, 1839 (2003).

[5] Phys. Rev. B **74**, 195202 (2006).

Speaker 2 (10:15 am - 10:50 am):

Mr. Linh Manh Nguyen (K57 Honor Program, Faculty of Physics, VNU University of Science)

Title: ***The transverse Ising model with arbitrary temperature***

Abstract: The Transverse Ising model was used to research the ferroelectric property of thin film materials. In this report, we use the differential technique to obtain some properties of lattice of spin ½ and, furthermore, the Monte Carlo method is used to study the phase transition of the lattice of spin ½ in 1-d.

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