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Stability and mobility of vacancy nanoclusters on Cu(111) surface: An *ab initio* study[1] ALIREZA AKBARZADEH, ZHENGZHENG CHEN, NICHOLAS KIOUSSIS, California State University Northridge, Deparment of Physics & Astronomy, 18111 Northridge, CA 91330-8268 — We used *ab initio* calculations to study stability and mobility of vacancy nanoclusters on Cu(111) surface. We found that the formation energies for single vacancies in the vicinity of surface are $\approx$0.3 eV lower than that in bulk. Interestingly, calculations yield strongly bonded 1^{st}NN divacancy on the surface than in bulk. In addition a trivacancy binds very strong on the surface, indicating that formation of loop-like vacancy nanoclusters are most energetically favored on the surface. These findings imply the ease of nucleation of vacancy nanoclusters on the surface. We also examined migration of mono-, di- and trivacancy on the surface. A zigzag motion for divacancy diffusion on the surface is predicted with the migration barrier higher on the surface than in the bulk due to larger binding energy and elastic contribution.

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