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**Effect of terrace width on site selectivity of C and S adsorption on stepped Pd surfaces** FAISAL MEHMOOD, SERGEY STOLBOV, TALAT S. RAHMAN, Department of Physics, Kansas State University, Manhattan KS 66502 — We have performed *ab initio* density functional theory calculations of C and S adsorption on stepped Pd surfaces to extract the role of terrace width on adsorption characteristics. Previous calculations<sup>1</sup> show that both C and S prefer to sit on hollow site between step edge and corner atom on Pd(211), although C atoms penetrate deeper into the surface and form much stronger bond with the neighboring Pd atoms. We present results here for C and S on Pd(533) which consist of 4-atoms wide terraces instead of 3 atoms on Pd(211). The trend in adsorption energies for C and S and the nature of the local bonding with the Pd atoms will be presented in detail along with the comparison between Pd(533) and Pd(211). Implications will be drawn for the relevance of the results to those for the Pd nanoparticles. This work is supported in part by NSF Grant No. CHE0205064, and by DOE under Grant No. DE-FGO3-03ER15445. <sup>1</sup>S. Stolbov, F. Mehmood, T. S. Rahman, M. Alatalo, I. Makkonen, and P. Salo, Phys. Rev. B **70**, 155410 (2004).

Talat Rahman  
Kansas State University

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