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By Cesare Pisani;Roberto Dovesi;Carla Roetti

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Title: Ab initio Hartree-Fock perturbed-cluster treatment of local defects in crystals: Authors: Pisani, C.; Dovesi, R.; Nada, R.; Kantorovich, L. N.

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Presentation "Fisica Torino 2014 Page 1 Quantum -

Fisica Torino 2014 Page 1 Quantum mechanical simulation of crystalline systems Quantum mechanical simulation of crystalline systems systems Roberto Dovesi

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Abstract. An ab-initio perturbed-cluster (PC) scheme is proposed for the treatment of the adsorption of isolated molecules on crystal surfaces. The PC equations are

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CRYSTAL is a quantum chemistry ab initio program, R. Dovesi, C. Roetti, R. Orlando, D Arco, and M. Llunell from Theoretical Chemistry Group at the

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