Abstract Submitted for the MAR12 Meeting of The American Physical Society

Density functional theory study of alkali doped picene MILAN TOMIC, HUNPYO LEE, ROSER VALENTI, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — We employ density functional theory methods to determine the equilibrium structures of  $A_x$  picene where A = Na, K, Rb, Cs and x = 1, 2, 3. We find that alkali doping with one, two and three alkali ions per picene molecule leads to subsequent filling of the LUMO and LUMO+1 derived bands of picene, leading to quarter, half and three quarter filled systems. We analyse the electronic structures using tight binding methods to derive the kinetic energy part of the underlying Hubbard Hamiltonian. As the interaction strength U on the picene molecules is expected to be large compared to the band width, we also employ manybody methods on the resulting Hamiltonian. We compare our results to photoemission experiments.

> Harald O. Jeschke Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany

Date submitted: 28 Nov 2011

Electronic form version 1.4