

Abstract Submitted
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Mott p-n junctions in layered materials¹ MAXIME CHARLEBOIS, Université de Sherbrooke, Québec, Canada, SYED HASSAN, RAJESH KARAN, The Institute of Mathematical Sciences C.I.T., Chennai, India, DAVID SENECHAL, Université de Sherbrooke, Québec, Canada, A.-M.S. TREMBLAY, Université de Sherbrooke, Québec, Canada and CIFAR, Canada — Correlated electron heterostructure became a possible alternative when thin film deposition techniques achieved structures with a sharp interface transition [1]. We study here the electronic reconstruction of doped Mott insulator p-n junctions based on a Cluster Dynamical Mean Field Theory (CDMFT) calculation of the Hubbard model in the limit where electrostatic energy dominates over the kinetic energy associated with transport across layers. The grand potential of individual layers is first computed within CDMFT and then the electrostatic potential energy is taken into account in the Hartree approximation. The charge reconstruction in an ensemble of stacked planes of different nature can lead to a distribution of electron charge [2], density of states, and optical properties that are unique to doped-Mott insulators.

[1] J. Mannhart, D. G. Schlom, *Science* 327, 1607 (2010)

[2] T. Oka, N. Nagaosa, *PRL* 95, 266403 (2005)

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