

Brainstorming Session for Impurities and Disorder with First Principles, UBC

October 3 – 7, 2011

Time	Monday	Tuesday	Wednesday	Thursday	Friday
9:30 – 10:30	DFT and downfolding related; also to substituted systems – dealing with rigid band, virtual crystal supercell Ole Krogh Andersen	The influence of impurities and disorder on superconductors including high Tc's and Pnictides Peter Hirschfeld	Determination of effective model Hamiltonian parameters including experimental methods. Intro to interactions and reductions due to various mechanisms and a few experimental methods George Sawatzky	Computational centre and a “conundrum” Mark Jarrell	Open discussion Session ends at 11:00 am
10:30 – 11:00	Coffee and discussions	Coffee and discussions	Coffee and discussions	Coffee and discussions	
11:00 – 12:30	Unfolding the electronic structure from folded zones and supercells using Wannier functions Wei Ku	Model methods and calculations to treat random impurities and disordered alloys including ways to determine the self energy; “Fermi surface” broadening in energy and momentum, Lindhard function and broadening of Nesting vectors. Maurits Haverkort	Model calculation of U and Hund's rule reductions in TM compounds Subhra Sen Gupta	s+- pnictide order parameter?? Or another related topic. Peter Hirschfeld	
12:30 – 13:30	Lunch break	Lunch break	Lunch break	Lunch break	
13:30 – 15:00	Another unfolding method with examples Maurits Haverkort / Ilya Elfimov	Configuration averaging methods and applications to NaxCoO2 and other systems Wei Ku	Resonant x ray scattering on the Manganites Hiroki Wadati	Bayo's exact diagonalization results on the cuprates and what that may mean for single band models George Sawatzky	
15:00 – 15:30	Coffee and discussions	Coffee and discussions	Coffee and discussions	Coffee and discussions	
15:30 – 17:00	Open discussion	Applications of configuration averaging and unfolding on the Fe Pnictides related to the question of doping vs. impurity scattering, comparison with rigid band, influence of nesting vector smearing etc. Ilya Elfimov/George Sawatzky	Cluster calculations on the Manganites Jochen Geck	Maurits Haverkort may want to say something about cluster DMFT?	