Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Total energy and force calculations for correlated materials[1] IVAN LEONOV, TP III, Center for Electronic Correlations and Magnetism, Uni Augsburg, Germany, VLADIMIR I. ANISIMOV, Institute of Metal Physics, Russian Academy of Sciences, Yekaterinburg, Russia, DIETER VOLLHARDT, TP III, Center for Electronic Correlations and Magnetism, Uni Augsburg, Germany — We present a computational scheme for the investigation of complex materials with strongly interacting electrons which is able to treat atomic displacements, and hence structural relaxation, caused by electronic correlations. It combines *ab initio* band structure and dynamical mean-field theory and is implemented with the linear response formalism regarding atomic displacements. We employ this approach to compute the equilibrium crystal structure and phase stability of a couple of correlated electron materials, such as elemental hydrogen, $SrVO_3$, and $KCuF_3$. Our results show an overall good agreement between the total energy and force computations of the equilibrium atomic position for these materials. The approach presented here allows one to study the structural properties of materials with strongly correlated electrons such as lattice instabilities observed at correlation induced metal-insulator phase transitions from first principles.

[1]We acknowledge support from the Deutsche Forschergemeinschaft through TRR 80 (I.L.) and FOR 1346 (V.I.A., D.V.).

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Date submitted: 09 Nov 2012 Electronic form version 1.4