Importance of electronic correlations for the phase stability of V_2O_3

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We report results for V_2O_3 obtained by a novel implementation of the LDA+DMFT approach for the computation of the total energy of materials with strongly interacting electrons. It includes a fully self-consistent calculation of the charge density, whereby correlation-induced changes in the effective Kohn-Sham Hamiltonian are taken into account. This scheme is employed to study the electronic structure and phase stability of V_2O_3 near a pressure-induced Mott-Hubbard metal-insulator transition. To explore structural transformations as a function of pressure, we use the experimentally determined atomic positions for the metallic and insulating phases, respectively, and calculate the total energy as a function of volume. We find that the structural stability depends very sensitively on changes of the lattice volume. In agreement with experiment, we observe that the metal-insulator transition is accompanied by a remarkable change of the c/a ratio. Full charge self-consistency is shown to be important to understand the phase stability of V_2O_3 near the Mott-Hubbard metal-insulator phase transition.