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Electron-phonon coupling and low-temperature structure of NaV_2O_5 JUERGEN SPITALER, Institute for Atomistic Modelling and Design of Materials,University Leoben, E. YA. SHERMAN, Department of Physics, University of Toronto, H.G. EVERTZ, Institute for Theoretical Physics, Graz Technical University, CLAUDIA AMBROSCH-DRAXL, Institute for Atomistic Modelling and Design of Materials,University Leoben, INSTITUTE FOR ATOMISTIC MODELLING AND DESIGN OF MATERIALS,UNIVERSITY LEOBEN TEAM, INSTITUTE FOR THEORETICAL PHYSICS, GRAZ TECHNICAL UNIVERSITY COLLABORATION — NaV_2O_5 is an extraordinary example of a structure where charge, spin and lattice degrees of freedom strongly interact. This low-dimensional compound is characterized by V atoms arranged in the form of ladders. At ambient conditions it is found to be quarter-filled with one electron distributed over one rung of the ladder. Going below $T_c = 34$K, NaV_2O_5 undergoes a phase transition involving a reordering of the V charges, a lattice deformation and a spin pairing. In order to investigate the mechanisms driving the phase transition, parameters of electron-phonon and spin-phonon for the Γ point phonons are determined from ab initio calculations within density functional theory. They are compared to the corresponding parameters of the isostructural CaV_2O_5, where no phase transition occurs. Moreover, ab initio results of several candidates for the low-temperature supercell of NaV_2O_5 are presented and analyzed in terms of total energies and electric field gradients.

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