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First principles investigation of the Fabre salts ANTHONY JACKO, ROSER VALENTI, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — The Fabre salts $(TMTTF)_2X$ are one dimensional charge transfer salts with a very rich phase diagram including charge ordered, Mott insulating, antiferromagnetic and spin Peierls phases. The structure involves stacks of TMTTF molecules with varying degree of dimerization. Open questions involve the role of the anions in the phase transitions. We investigate the electronic structure of compounds with a number of different anions like $X = AsF_6$, PF_6 and Br. We discuss the properties of the underlying Hubbard Hamiltonian for these materials.

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