Lattice and transport properties of the misfit-layered oxide thermoelectric $Ca_3Co_4O_9$ from first principles ALEJANDRO REBOLA, ROBERT KLIE, University of Illinois at Chicago, PETER ZAPOL, Argonne National Laboratory, SERDAR OGUT, University of Illinois at Chicago — The misfit-layered oxide $Ca_3Co_4O_9$ (CCO) has recently been the subject of many experimental and some theoretical investigations due to its remarkable thermoelectric properties. CCO is composed of two incommensurate subsystems, a distorted rocksalt-type Ca_2CoO_3 layer sandwiched between hexagonal CoO_2 layers. Taking into account that the composition ratio between these subsystems is very close to the golden mean, which is the limit of the sequence of the ratios of consecutive Fibonacci numbers $F(n)$, we model CCO from first principles[1] by using rational approximants of composition $[Ca_2CoO_3]_{2F(n)}[CoO_2]_{2F(n+1)}$. In the present study, we use 3/2 and 5/3 rational approximants and PBE+U computations to calculate the *ab initio* phonon dispersion curves, related thermal properties, as well as *ab initio* electronic transport properties such as DC conductivity and thermopower within the relaxation time approximation by applying the Boltzmann transport theory. Results are compared with available experimental data and potential routes for increasing the thermopower of CCO are discussed.

[1]A. Rebola, R. F. Klie, P. Zapol, and S. Ogut, Phys. Rev. B **85**, 155132 (2012)

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