

Pemodelan dan perhitungan konduktivitas optis pada layered $\text{Pr}_0.5\text{Ca}_1.5\text{MnO}_4$ dengan dynamical mean field theory = Modelling and calculations of optical conductivity of layered $\text{Pr}_0.5\text{Ca}_1.5\text{MnO}_4$ within dynamical mean field theory

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Abstrak

Kami melakukan perhitungan konduktivitas optis pada layered (perovskite) $\text{Pr}_0.5\text{Ca}_1.5\text{MnO}_4$ untuk mengidentifikasi fenomena charge-ordering. Pemodelan melibatkan orbital Mn dan O yang berada pada bidang MnO_2 dari layered $\text{Pr}_0.5\text{Ca}_1.5\text{MnO}_4$. Interaksi yang diperhitungkan dalam pemodelan yaitu interaksi Coulomb inter-orbital dan intra-orbital, distorsi Jahn-Teller dan exchange interaction dengan menerapkan beberapa asumsi. Perhitungan dilakukan menggunakan Dynamical Mean Field Theory untuk mencapai self-consistency. Hasil perhitungan menunjukkan profile yang mendekati hasil eksperimen dengan puncak charge-ordering berada di bawah 1 eV dan puncak charge-transfer pada 3-3.7 eV. Di bawah temperatur $\text{TCO}=\text{OO}$ (325 K), puncak charge-ordering mengalami blue shift seiring dengan penurunan temperatur.

<hr><i>We calculate the optical conductivity of layered (perovskite) $\text{Pr}_0.5\text{Ca}_1.5\text{MnO}_4$ to capture charge-ordering phenomena. The calculations are based on a model which considers Mn and O orbitals within the MnO_2 plane of layered $\text{Pr}_0.5\text{Ca}_1.5\text{MnO}_4$. Interaction terms included in the model with some assumptions are the inter-orbital and intra-orbital Coulomb repulsions, the static Jahn-Teller distortion and the exchange interaction. We calculate within Dynamical Mean Field Theory to achieve self-consistency. The result shows a profile similar to recent experimental data, where the charge-ordering peak appears below 1 eV and charge-transfer peak at 3-3.7 eV. For temperature lower than $\text{TCO}=\text{OO}$ (325 K), the charge-ordering peak undergoes a blue shift as the temperature is decreased.</i>