Pemodelan dan perhitungan konduktivitas optis pada layered pr0 5ca1 5mno4 dengan dynamical mean field theory = Modelling and calculations of optical conductivity of layered pr0 5ca1 5mno4 within dynamical mean field theory

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Abstrak

Kami melakukan perhitungan konduktivitas optis pada layered (perovskite) Pr0.5Ca1.5MnO4untuk mengidentifikasi fenomena charge-ordering. Pemodelan melibatkan orbital Mn dan O yang berada pada bidang MnO2 dari layered Pr0.5Ca1.5MnO4. 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 TCO=OO (325 K), puncak charge-ordering mengalami blue shift seiring dengan penurunan temperatur.
<hr>We calculate the optical conductivity of layered (perovskite) Pr0.5Ca1.5MnO4 to capture charge-ordering phenomena. The calculations are based on a model which considers Mn and O orbitals within the MnO2 plane of layered Pr0.5Ca1.5MnO4. 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 temperaturelower than TCO=OO (325 K), the charge-ordering peak undergoes a blue shift as the temperature is decreased.