Pemodelan dan perhitungan pada single layered pr-0.5ca-1.5 mno-4 untuk menjelaskan fenomena keteraturan muatan dan orbital dan manifestasinya pada konduktivitas optis = Modeling and computation of single layered pr-0.5ca-1.5mno-4 to explain charge and orbital ordering phenomena and their manifestation in optical conductivity

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Abstrak

Kami melakukan perhitungan konduktivitas optis pada layered (perovskite) Pr0.5Ca1.5MnO4 untuk 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.

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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 temperature lower than TCO/OO (~325 K), the charge-ordering peak undergoes a blue shift as the temperature is decreased.