**Article:**[**Study the Pollutants Chlorophenols: Electronic and Physical Properties Relationship**](https://www.researchgate.net/publication/307973582_Study_the_Pollutants_Chlorophenols_Electronic_and_Physical_Properties_Relationship?ev=prf_pub)

[Abdul Hameed M Jawad Al Obaidy](https://www.researchgate.net/profile/Abdul_Hameed_Al_Obaidy) · [Ahmed Al-Amiery](https://www.researchgate.net/profile/Ahmed_Al-Amiery) · [Rana Al-Ani](https://www.researchgate.net/profile/Rana_Al-Ani)

**ABSTRACT:** Geometrical optimization and electronic structure of chlorophenols were researched by DFT (B3LYP) utilizing a 3-21G basis set. We have likewise researched the aggregate electronic properties, Highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) and energy gap. The calculated HOMO and LUMO energies demonstrate that charge transfer occurs within the molecule.

Article · Jan 2016