

بسم الله الرحمن الرحيم

قال تعالى: (لِلَّهِ مُلْكُ السَّمَاوَاتِ وَالْأَرْضِ وَمَا فِيهِنَّ لَهُوَ عَلَى كُلِّ شَيْءٍ
قَدِيرٌ)
المائدة الآية (120)

صدق الله العظيم.

Dedication

I dedicate to my beloved mother for all the
....sacrifices she has given to my life

To the soul of my father who dreamt of the day
...of my graduation, god bless him in heaven

Special thanks to my dearest sisters, Husna
.and Fatima, my brothers and colleagues

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Abstract

In this research we used the first-principles calculations to study the electronic structure of the face center cubic (FCC) calcium chloride (CaCl_2); using pseudopotential approach (as implemented by the QANTUM ESPRESSO package). We found the charge density, density of states and .energy band gap for the FCC CaCl_2

النتائج

في هذا البحث تم استخدام المبادئ الأولية في دراسة التركيب الإلكتروني لمركب كلوريد الكسيوم متمركز الأوجة; وذلك باستخدام الجهد الفعال كأداة في برامج حزمة (QANTUM ESPRESSO).

ولقد وجدت نطاقات الطاقة والتي من خلالها تم حساب فجوة الطاقة ; كما وجدت ايضا كثافة الحالات.

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