بسم الله الرحمن الرحيم

قال تعالي: (**لِلَّهِ مُلْكُ السَّمَاوَاتِ وَالْأَرْضِ وَمَا فِيهِنَّ ۚ وَهُوَ عَلَىٰ 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 psedopotintial approach (as implemented by the QANTUM ESPRESSO package). We found the charge density, density of states and .energy band gap for the FCC $CaCl_2$

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

ول قد وجدت نطا قات الطا قة والتي من خلالها تم حساب فجوة الطا قة ;كما وجدت ايضا كثافة الحالات.

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