

الآية

قال تعالى:

اللّٰهُ أَنْزَلَ مِنَ السَّمَاءِ مَاءً فَأَخْرَجْنَا بِهِ ثَمَرَاتٍ مُّخْتَلِفًا أَلْوَانُهَا وَمِنَ الْجِبَالِ جُدَدٌ بَيضٌ وَحُمْرٌ مُّخْتَلِفٌ وَأُخْرٌ أَبْيَضٌ كَالْبُهَيْمِ نُودًى (28) النَّاسِ وَالذَّوَابِّ تَلْفُؤْ أَلْوَانًا كَمِثْلِ الْغَدَقِ إِنَّمَا يَخْشَى اللَّهَ مِنْ عِبَادِهِ الْعُلَمَاءُ إِنَّ اللَّهَ عَزِيزٌ غَفُورٌ (28)

سورة فاطر

Dedication

To my mother.....My first teacher

To my father.....My hero

To my brothers, sisters

To my friends

To all those unbelievable persons

I am trying to say thank you

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Abstract

The studies of zinc oxide doped by strontium were carried out using first principles calculations under the density functional theory(DFT), including the hybrid functional Beck's B3LYP functional and was performed using CRYSTAL06 program.

Initial investigation were made on the parent ZnO with supercell 2x2x1. The results calculations were found to agree with experimental data.

Calculations have been made to study the electrical properties of zinc oxide when it doped with different percentage of strontium atoms.

On substitution one Zn by Sr, we found that the band energy decreased to the value 3.28 eV which means improve in the electrical conductivity of the compound. We found also that when the dopant increases the band energy increases too.

Finally, accordingly, we predict that this new compound will have many optical applications.

المستخلص

لقد أجريت الدراسة علي مادة أكسيد الزنك عندالتشويب بالمادة الاسترانيشومبالنسبة تشويب مختلفة مكونة المركب $Sr_xZn_{x-8}O_8$ باستخدام حسابات المبادئ الأولية التي تعتمد علي نظرية الكثافة الدالية متضمنة الدالية المهجنة B3LYP بإستخدام برنامج CRYSTAL06.

الدراسات الأولية علي المركب الرئيسي ZnO أظهرت أن النتائج الحاسوبية متوافقة مع النتائج التجريبية مع هذا المركب.

أجريت الحسابات لدراسة خواص الكهربائية ولقد وجد أن عند نسبة التشويب 12.5% تقل فجوة الطاقة إلى قيمة 3.28 eV وتزداد بزيادة نسبة التشويب تدريجيا مما يدل علي زيادة مقاومه المادة عند أضافه التزايد لمادة الاسترانيشوممع التنبؤ بتغير في الخواص البصرية للمركب المشويب .

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