عنوان مقاله:

Development of Exchange and Correlation Functional in DFT Method by C++ Program

محل انتشار:

همایش منطقه ای شیمی (سال: 1389)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Exchange and Correlation functional is one of the best important of energy for a system. In this work we have developed it and created a new functional for calculating energy for a system. We have built a new functional by C++ program and quantum mechanics calculation to achieve it. We have made to effort using many simple systems to fitting our result. We have used Gaussian 98 Code for calculation and Hyper Chem Code for drawing structure of systems. In this work we have utilized of some hybrid methods (B3LYP, BLYP, PBE...) and many basis sets such as 6-31G* , 6-31G** , MPn,…. We have called our new functional KMFLYP. KMF section indicates exchange functional .and LYP section indicate correlation functional. Our results show a good agreement to experimental results

کلمات کلیدی: