

عنوان مقاله:

Application of Modern Computers in in-silico Chemical Simulations

محل انتشار:

بیست و ششمین سمینار شیمی آلی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

With the recent advances in computer hardware and programming codes for running quantumchemical and molecular dynamics simulations in a massively parallel manner, the in-silicotools have become a reality for modeling chemical systems of interest [1]. The software packages are becoming more advanced and intuitive. Their documentation has become very easy to follow and their graphical user interface, in some cases is so user-friendly that not much coding or quantum background is required for running simulations [2]. This provides an opportunity for the experimental chemical community to use these tools on a daily basis for exploring their systems. This project provides some examples of the application of quantumchemical calculations.

کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا:

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