Geometry Global Optimization of Large Biological Molecules

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One presents a methodology to find the global minimum of a material system (molecule, cluster, bulk) on the potential energy surface (PES) which is its fundamental geometrical configuration (native state for proteins for example). The idea is to compute data at quantum level and to use them to determine a classical inter-atomic potential, which will be used to optimize the geometry of the system. One introduces first the mathematical background of the so-called order N or linear-scaling algorithms[1] which permit *ab initio* calculations within Density Functional Theory framework (Kohn-Sham), of large material systems such as biological molecules for instance. In a second step, the symbolic regression method is introduced in order to determine the inter-atomic potential with mean of genetic programming which is a generalization of genetic algorithm[2]. This permits in third step to use it for the Minima Hopping method[3, 4], which performs global optimization on the PES. The presentation ends with some examples of numerical applications.

References

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