Global Approach to Fast and Accurate Learning of Potential Energy Surfaces and Forces of Small Organic Molecules

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Application of Statistical learning to physical and chemical problems is becoming a popular tool due to availability of large quantum mechanical reference datasets and increasing computational resources. We show how in principle it is possible to learn potential energy surfaces and atomic forces of different small organic molecules from ab initio molecular dynamics reference calculations. Representing the different molecules by Coulomb Matrix descriptor, we assess the performance of this statistical learning model for relative small training set of ab initio molecular dynamics reference calculations. At relatively small computational cost, cross-validation over ten thousands molecular dynamics configurations yields mean absolute errors smaller than 1 kcal/mol (chemical accuracy). Furthermore we propose two new fast and efficient methods based on this model for predicting atomic forces within density functional theory (DFT) calculations accuracy in a global approach which does not require complicated local atomic coordinates set up or machine learning force fields which lack of transferability.