Exploring Structure and Dynamics of Large PAHs clusters using Deep Neural Network Potentials

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Abstract:

Since the 1970s, characteristic emission features known as Aromatic Infrared Bands (AIBs) have been observed throughout the Interstellar Medium (ISM). These bands are widely attributed to Polycyclic Aromatic Hydrocarbons (PAHs), which are now estimated to account for 10% to 20% of the galactic carbon. Consequently, PAHs play a fundamental role in key astrophysical processes, such as the formation of molecular hydrogen (H_2) or the photoelectric heating of interstellar gases. In the ISM, these molecules exist in various forms, notably as pure or mixed clusters (incorporating different PAH species or other molecules like water). To study these systems theoretically, density functional based tight binding (DFTB), a semi-empirical formulation of DFT, has emerged as a method of choice, particularly for clusters containing around a hundred atoms[1]. However, DFTB alone remains insufficient to fully characterize the thermodynamic and structural properties of larger and more realistic clusters that can reach up to a thousand atoms.

To overcome this limitation, deep neural network potentials (DNNPs) have emerged as a promising approach to achieve both high accuracy and low computational cost[2]. By implementing an efficient active learning procedure, we have developed DNNPs that maintain DFTB level quality for clusters of several hundred atoms as illustrated in Figure 1. This approach enables a complete description of these complex systems, bridging the gap between molecular scales and "very small grains". We will present preliminary results. The challenge for these systems is the transferability of the DNNP with size and the good description of anisotropic interactions of various nature.

Keywords: Polycyclic Aromatic Hydrocarbons, Clusters, Deep Neural Network Potentials

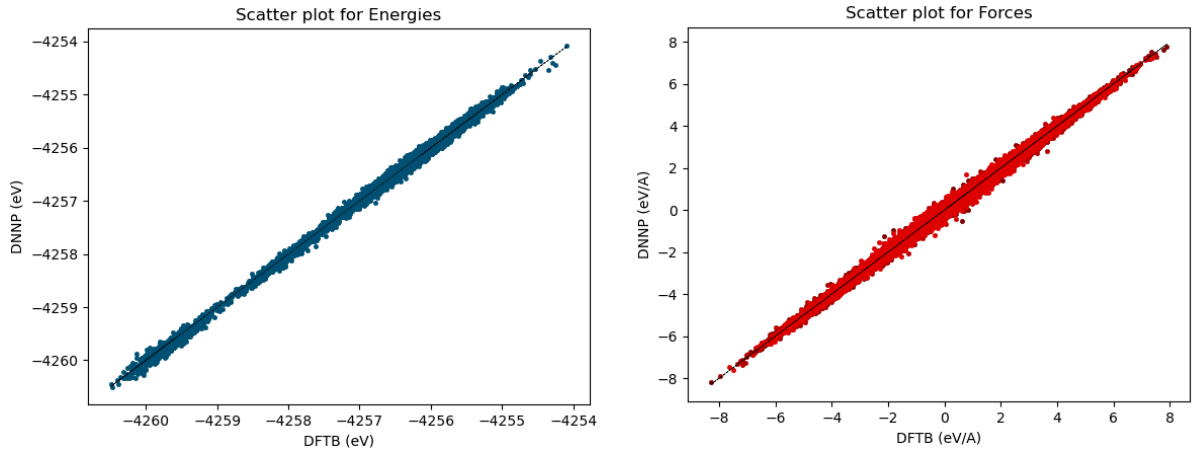

Figure 1. Correlation plots of energies and forces for $(C_{16}H_{10})_5$.

References:

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