General-purpose ML interatomic potential for CH and CHO: unifying the description of organic materials and molecules

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Organic compounds composed of carbon, hydrogen, and oxygen (CHO) are essential building blocks of life and are fundamental to biochemistry, medicine, environmental science, and a multitude of industrial applications. Their remarkable versatility stems from carbon's unique bonding capabilities, enabling the formation of a diverse array of complex structures and functional groups.

Understanding the microscopic properties of organic materials is increasingly critical for establishing precise links between fabrication conditions and the resulting properties and performance in applications. Because accessing detailed interatomic interactions experimentally remains challenging, this limitation highlights the need for a unified computational framework capable of capturing these interactions comprehensively across diverse conditions. In this talk, we will explore the exciting possibilities that machine learning (ML) presents for constructing interatomic potentials or ML potentials (MLPs) for a comprehensive description of organic materials within a single model.

To begin, I will present our developed general-purpose CH MLP [1] using Gaussian Approximation Potential (GAP) and how the potential describes different problems, such as the formation of simple and complex alkanes, aromatic hydrocarbons, hydrogenated amorphous carbon (a-C), and CH systems under extreme conditions. I will show how we use this model to generate hydrocarbons of different sizes and complexities without prior knowledge of organic chemistry rules, capturing the relationships and transformations between hydrocarbons and hydrogenated carbon materials across various conditions within a single computational framework. Next, I will demonstrate how we can expand this potential to enable simulations of a broader range of organic materials composed of C, H, and O, including organic molecules, cellulose, and its derivatives [2].

Figures

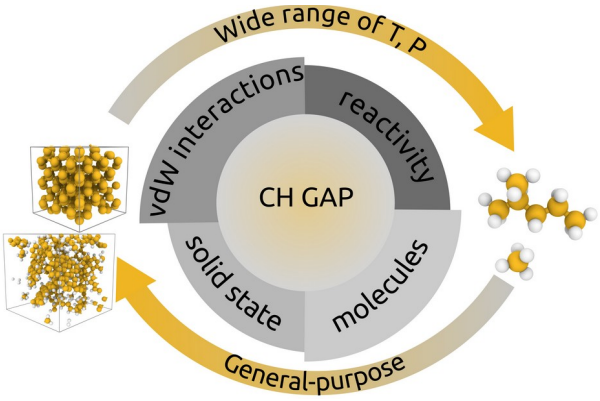

Figure 1. Schematics of different components of CH GAP.

References

[1] R. Ibragimova, M.S. Kuklin, T. Zarrouk, and M.A. Caro, Chemistry of Materials, 37(3) (2025) 1094.
[2] T. Zarrouk, R. Ibragimova, A.P. Bartók, and M.A. Caro. J. Am. Chem. Soc. 146 (2024) 14645.