Many-body dispersion from machine learning for molecules and materials

Evgeny Moerman[1], Adil Kabylda[1], Almaz Khabibrakhmanov[1], Alexandre Tkatchenko[1]
[1]Université du Luxembourg, 162a, Avenue de la Faïencerie, Luxembourg, Luxembourg

evgeny.moerman@uni.lu

Van der Waals (vdW) interactions are essential for describing molecules and materials, from drug design and catalysis to battery applications [1,2,3]. These omnipresent interactions must also be accurately included machine-learned force fields. The many-body dispersion (MBD) method [4] stands out as one of the most accurate and transferable approaches to capture vdW interactions, requiring only atomic C_6 coefficients and polarizabilities as input. We present MBD-ML, a message passing neural network that predicts these atomic properties directly from atomic structures. Through seamless integration with libMBD, our method enables the immediate calculation of MBD-inclusive total energies, forces, and stress tensors. By eliminating the need for intermediate electronic structure calculations, MBD-ML offers a practical and streamlined tool that simplifies the incorporation of state-of-the-art vdW interactions into any electronic structure code, as well as empirical and machine-learned force fields.

References

[1] J. Hermann, R. A. DiStasio Jr., and A. Tkatchenko, Chemical Reviews, 6 (2017) 4714 - 4758.
[2] T. Björkman, A. Gulans, A. V. Krasheninnikov and R. M. Nieminen, Journal of Physics: Condensed Matter, 24 (2012) 424218 - 424228.
[3] E. B. Isaacs, S. Patel, C. Wolverton, Physical Review Materials, 4 (2020) 065405-1 - 065405-11.
[4] J. Hermann, A. Tkatchenko, Physical Review Letters, 124 (2020) 146401-1 – 146401-7.
[5] S. Ganscha, O. T. Unke, D. Ahlin, H. Maennel, S. Kashubin, K-R Müller, Scientific Data, 406 (2025), 1-15.

Figures

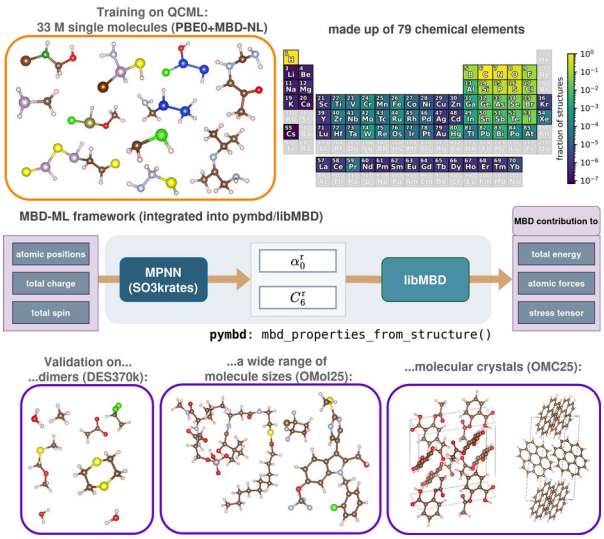

Figure 1. MBD-ML workflow and overview over training data and the chemical compound spaces the model was validated on. Top right figure reproduced from Ref. [5] under CC BY 4.0,