Mie-FH: A Quantum-corrected Potential in LAMMPS Simulation Package

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The accurate modeling of interatomic interactions in molecular dynamics simulations is crucial for understanding the properties of materials at the nanoscale. We introduce a novel implementation of quantum-corrected Mie potential (Mie-FH) [1] into the popular Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package. This potential is designed to provide a more precise description of the interaction energies and forces between particles, particularly in systems where quantum effects might play a significant role.

In order to demonstrate the effectiveness of our new implementation, we have applied it to study hydrogen and helium gas, two prototypical molecular systems where quantum effects are known to play a crucial role. Our results show that Mie-FH provides an accurate description of the interaction energies and forces in these systems. Furthermore, we have conducted extensive benchmarking tests to assess the computational efficiency of our new implementation, revealing that Mie-FH can be used with confidence for large-scale simulations involving millions of particles. The code will be published on our github repo [2].

References

1. Aasen, A., Hammer, M., Ervik, Å., Müller, E. A., & Wilhelmsen, Ø. (2019). Equation of state and force fields for Feynman–Hibbs-corrected Mie fluids. I. Application to pure helium, neon, hydrogen, and deuterium. *The Journal of Chemical Physics*, *151*(6).
2. https://github.com/thermotools/