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Van der Waals Interactions in Pyridine and Pyridine-like Molecular Crystals: An *ab initio* Molecular Dynamics Study[1] HSIN-YU KO, ROBERT A. DISTASIO JR., BISWAJIT SANTRA, ROBERTO CAR, Princeton Univ — Pyridine has recently been investigated as a potentially effective material for use in artificial light harvesting.[2] In this work, we propose the use of *ab initio* molecular dynamics (AIMD) to gain valuable physical insight into the artificial photosynthetic processes occurring in condensed-phase pyridine, the study of which has been limited to semi-empirical force fields to date.[3] For this purpose, we introduce an accurate and efficient AIMD method, based on density functional theory (DFT) and a self-consistent pairwise description of van der Waals (vdW) interactions, for use in finite temperature and pressure (NPT) simulations on pyridine and several pyridine-like molecular crystals (PLMCs). Utilizing this approach, we demonstrate that vdW forces play a crucial role in the theoretical prediction of the structure and density of pyridine and PLMCs, and therefore must be accounted for in studies of these potential alternative energy materials.

[1]DOE: DE-SC0008626, NSF: DMS-1065894
[2]EB Cole, PS Lakkaraju, DM Rampulla, AJ Morris, E Abelev, AB Bocarsly J. Am. Chem. Soc., **132**, 11539 (2010).
[3]AT Anghel, GM Day, SL Price CrystEngComm., **4**, 348 (2002).

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