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**Linear Scaling First-Principles Molecular Dynamics with Plane Waves accuracy**[1] JEAN-LUC FATTEBERT, Lawrence Livermore National Laboratory, Livermore, CA 94551, FRANCOIS GYGI, UC Davis, Davis, CA 95616 — As an alternative to the Plane Waves (PW) approach for highly accurate and unbiased Density Functional Theory molecular dynamics simulations with pseudopotentials, we propose to use a real-space finite differences discretization and a localized orbitals representation of the electronic structure. As in the PW approach, the discretization error can be reduced systematically by decreasing the mesh spacing, while the truncation error due to orbitals localization constraints decreases exponentially with the size of the localization regions. Accurate atomic forces can be computed and allow microcanonical molecular dynamics simulations. Using a supercell of 512 water molecules, we demonstrate an excellent energy conservation for localization regions large enough. We propose an explanation for the negative energy drift observed for smaller radii based on the presence of local minimas. Our implementation demonstrates an effective scaling complexity close to linear with the system size and a good parallel scaling with the number of processor

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