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Direct Determination of Electric Current in Born-Oppenheimer Molecular Dynamics[1] TAO SUN, RENATA M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science, University of Minnesota — We introduce a new approach to calculate directly the electric current in Born-Oppenheimer molecular dynamics. In this approach the electric current is computed from the adiabatic variations of the Kohn-Sham eigenstates between consecutive time steps. This conceptually straightforward method is fairly efficient and can be easily implemented into existing electronic structure programs. We test the method in two representative systems: liquid D_2O and crystalline MgO. The polarization change and the electric current density computed from the present approach are in excellent agreement with those from the Berry phase method and explicit density functional perturbation theory calculations of Born-effective charges.

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