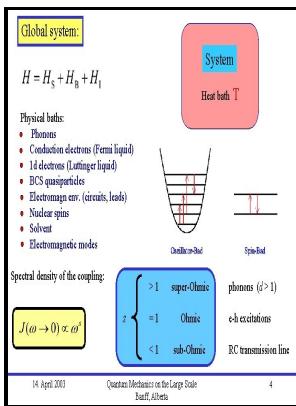


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In classical Newtonian MD, the motion of atom or molecule particles is based on the empirical or effective interaction potentials, which in turn can be based on curve-fit of ab initio calculations or curve-fit to thermophysical properties. . ACS Nano 2019, 13 12 , 13658-13667.

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Phys. Rev. B 58, 15557 (1998)

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