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### **Theory of Molecular Dynamics Simulations**

These partial charges are stationary with respect to the mass of the atom. But molecular dynamics simulations can explicitly model polarizability with the introduction of induced dipoles through different methods, such as Drude particles or fluctuating charges. This allows for a dynamic redistribution of charge between atoms which responds to the local chemical environment.

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### **Molecular Dynamics Simulation | Guide books**

Two textbooks on molecular dynamics are, J.M. Haile, "Molecular Dynamics Simulations: Elementary Methods", Wiley, New York (1992) Google Scholar D.C. Rapaport, "The Art of Molecular Dynamics Simulation", Cambridge University Press, Cambridge, England (1995) Google Scholar

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