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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.

Molecular dynamics - Wikipedia

more quickly in simulation, or making the simulation reach all low-energy conformational states more quickly. - For example, one might apply artificial forces to pull a drug molecule off a protein, or push the simulation away from states it has already visited. - Each of these methods is effective in certain specific cases.!

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