MD BY X-RAYS?

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By the equipartition theorem, MD assumes heating a molecule increases the temperature of the atoms that is converted to their momenta causing the vibrational motion of atoms, the changes in atomic positions initiating chemical reactions. However, the Planck law of QM precludes any increase in atom temperature because the heat capacity of the atom vanishes under the EM confinement induced by their high surface-to-volume ratios. QM stands for quantum mechanics.

Lacking heat capacity by QM, molecular heat is proposed conserved in atoms by QED creating EM radiation having half-wavelength $\lambda/2 = d$ standing across their diameter d. QED here is a simple form of the complex light-matter interaction proposed by Feynman and others. Simple QED in atoms creates X-rays having Planck energy $E = hv$, where h is Planck's constant and v is frequency, $v = (c/n) / \lambda$ and c and n are the velocity of light and the refractive index of the atom. At X-ray frequencies, $n = 1$. Hence, colloidal gold atoms having $d = 288$ pm produce X-rays having $E = 2.2$ keV.

Recently, study[1] shows RIXS may be tuned to excite specific types of vibrational motion, e.g., X-ray photons can be tuned to symmetric stretching while other tunings excite bending modes. RIXS stands for resonant inelastic X-ray scattering spectroscopy. This is significant as chemical reactions need not be initiated by thermally induced changes in atom positions, but rather by X-rays, especially since temperatures in atoms are precluded by QM.

Vibrational control of atoms by X-rays makes MD simulations based on the equipartition theorem problematic. Modifications to MD consistent with QM are presented.

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1. R. C. Couto, et al., "Selective gating to vibrational modes through resonant X-ray scattering," Nature Communications, 8, 14165/DOI: 10.1038/ncomms14165.