To Whom It May Concern:
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My previous experience with molecular dynamics is as an advisor to two students on their Ph.D. Thesis: (i) Silvina Tomasone published from Northeastern University in Physical Review Letters and (ii) Duccio Medina published from the University of Perugia in the Journal of Chemical Physics.

Silvina performed Molecular dynamics computations for noble gas atoms, say argon, adsorbed as a sub-monolayer film on the metal plates of a quartz oscillator microbalance. The oscillator frequency shift and width of the microbalance mode in theory agreed satisfactorily with molecular dynamics theory. But this would not be true for adsorbed films of water.

The point in my mind is that due to the water dipole-dipole potential

$$U_{12} = \frac{\mathbf{d}_1 \cdot \mathbf{d}_2 R^2 - 3(\mathbf{d}_1 \cdot \mathbf{R})(\mathbf{d}_2 \cdot \mathbf{R})}{R^5} \qquad \text{wherein} \qquad \mathbf{R} = \mathbf{r}_1 - \mathrm{r}_2$$

being too long ranged for classical molecular dynamics computation to be in agreement with experiment. Thus, molecular dynamics will not agree with experiment for water sub-monolayer films. The only experimental evidence I know about for the adsorption of a water monolayer on metal films is that of my at one time collaborator Jackie Krim when she was at Northeastern University. She found anomalous experimental results that she refused to show anybody including me. The importance of the adsorption physics to the covid-19 virus medical treatments is that at least for viruses previous to the delta variety, a corona virus adsorbed on a metal lives only a few hours while a corona virus in bulk insulting material lives for a few days. Thus, some metal threads in insulating cloth facemasks are often employed shortening the virus lifetime.

More to the point of biological physics, Duccio performed molecular dynamics to explain deep inelastic neutron scattering from Azurin protein that Duccio obtained in his experiment at the pulsed neutron facility in Grenoble France. Because the proton and neutron have a shallow nuclear bound state, i.e. the deuteron, the scattering length in neutron-proton scattering is anomalously large so that the “parton” in the protein for “deep inelastic neutron” scattering is the proton. Thus the cross section per unit volume of protein for neutron momentum and energy transfer, respectively,

$$\hbar\mathbf{Q} = \mathbf{p}_i - \mathbf{p}_f \qquad \text{and} \qquad \hbar\omega = \varepsilon_i - \varepsilon_f ,$$

is thereby

$$\frac{d^2h}{d\Omega d\omega} \approx \frac{d\sigma}{d\Omega}\left[2\int n(\mathbf{p})\delta\left(\omega - \frac{\mathbf{Q}\cdot\mathbf{p}}{M} - \frac{\hbar Q^2}{2M}\right)\frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\right]$$

wherein $n(\mathbf{p})$ is the momentum occupation number of the protons in the protein.

Numerical Analysis Theorem:

The momentum distribution in any molecular dynamics computation with a theoretical thermostat at temperature T is the Maxwell occupation. Foe classical molecular dynamics,

$$n(\mathbf{p}) \propto \exp\left(-\frac{p^2}{2Mk_BT}\right) \quad \rightarrow \quad \left\langle p^2 \right\rangle = 3Mk_BT$$

Experimental Results for Protons:

In pure water and for proteins, the proton momentum distribution as measured by deep inelastic neutron scattering is too broad to be Maxwell. Experimentally, classical molecular dynamics ***fails*** for protons in protein biological matter. **Quantum mechanics is required for protons and thereby for electric dipole moments. This also holds true for protons in DNA (bacteria) and RNA (viruses).**

Allan Widom