New Interpretation of NMR Relaxation Response from MD Simulations: Material Properties and MRI Contrast Agents

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Nuclear magnetic resonance (NMR) relaxation has emerged as an essential tool in probing matter non-destructively with applications spanning materials, energy, and medicine. Interpreting the NMR relaxation response has previously depended on idealized models. In this work, we describe the new scientific approach of interpreting NMR relaxation response using molecular dynamics simulation, without assuming any relaxation model or adjustable parameter. This work has resolved certain paradoxes in the field and it potentially enables enhanced interpretation of NMR relaxation and development of new applications as well as new MRI contrast agents.

At high NMR frequencies, quantum effects make a negligible contribution to the total Hamiltonian of the system, and one can investigate NMR relaxation at such conditions using classical Molecular Dynamics (MD) simulations. We have used classical MD simulations to calculate T1 and T2 for bulk hydrocarbons and water; the results agree very well with measurements, but disagree with traditional theories of relaxation that make severe assumptions about molecules and their interactions. Studies on polymeric liquids and the glass-former glycerol across a range of temperatures again show good agreement with experiments, but challenge traditional theories of relaxation. Importantly, for the polymeric liquids, we find that the enhanced NMR relaxation observed in these systems is due to confinement, not paramagnetism as commonly assumed. Our studies on the NMR relaxation of water hydrogen protons in the presence of gadolinium(III), a well-known element used in MRI contrast agents, shows that the relaxation can be captured at human body temperature and at usual MRI frequencies, opening a new avenue for enhancing the interpretation of MRI without relying on traditional theories of relaxation.