Microsymposia

MS.89.5

Active Data Dictionaries: A Future Role for DDLm
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A 2009 editorial Data’s Shameful Neglect in Nature (461, pp 145) and several accompanying articles drew attention to the scandalous shortfall in data sharing between researchers. It highlighted the lack of technical, institutional and cultural frameworks for supporting open data access and archiving.

The crystallographic community recognised these issues 20 years ago and developed a Crystallographic Information Framework (CIF) which is now the mainstay of all open data access, exchange and archiving, at least within structural chemistry. The submission of experimental and model data is mandated for all publications of the IUCr, for data deposition to the PDB and several chemical databases.

The CIF is a subset of the STAR format, the latest version of which was presented at the 2008 IUCr Osaka Congress as the basis for a new CIF formalism. Extensions to STAR facilitate the active dictionary definition language DDLm that can extend dictionary definitions via dREL-based methods.

This paper will review the underpinning syntactic and structural simplicity of STAR. We will show that semantically rich definitions are possible through an active dictionary definition language that supports an expandable range of data types and functions, and invokes the full scope of dREL-methods capabilities.

Keywords: STAR, CIF, DDL

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Quantum nature of the hydrogen bond
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Hydrogen bonds are weak, generally intermolecular bonds, which hold much of soft matter together as well as the condensed phases of water, network liquids, and many ferroelectric crystals. The small mass of hydrogen means that they are inherently quantum mechanical in nature, and effects such as zero-point motion and tunneling must be considered, though all too often these effects are not considered.

As a prominent example, a clear picture for the impact of quantum nuclear effects on the strength of hydrogen bonds and consequently the structure of hydrogen bonded systems is still absent. Here, we report ab initio path integral molecular dynamics studies on the quantum nature of the hydrogen bond. Through a systematic examination of a wide range of hydrogen bonded systems we show that quantum nuclear effects weaken weak hydrogen bonds but strengthen relatively strong ones. This simple correlation arises from a competition between anharmonic intermolecular bond bending and intramolecular bond stretching. A simple rule of thumb is provided that enables predictions to be made for hydrogen bonded materials in general with merely classical knowledge (such as hydrogen bond strength or hydrogen bond length).

Our work rationalizes the influence of quantum nuclear effects, which can result in either weakening or strengthening of the hydrogen bonds, and the corresponding structures, across a broad range of hydrogen bonded materials [1-3]. Furthermore, it highlights the need to allow flexible molecules when anharmonic potentials are used in force field-based studies of quantum nuclear effects.

Keywords: hydrogen bonds, density functional theory, path integral molecular dynamics

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Quantum protons in hydrogen bonds
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The momentum distribution of the protons participating in hydrogen bonds in water and ice deviates considerably from the classical equilibrium distribution. As a consequence the molecular structure of water and ice is directly affected by quantum mechanics [1]. Yet the effect is essentially quasi-harmonic and quasi-classical in nature [2]. New physics arises in presence of proton tunneling, which is collective and dominated by strong local correlations.

Keywords: hydrogen bond, scattering, quantum phase transition