Abstract Submitted
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Neutron Scattering in Chemistry: Experiments, Models and Statistical Description of Physical Phenomena[1] TIMMY RAMIREZ CUESTA, Oak Ridge National Lab — Incoherent inelastic neutron scattering spectroscopy is a very powerful technique that requires the use of ab-initio models to interpret the experimental data. Albeit not exact the information obtained from the models gives very valuable insight into the dynamics of atoms in solids and molecules, that, in turn, provides unique access to the vibrational density of states. It is extremely sensitive to hydrogen since the neutron cross section of hydrogen is the largest of all chemical elements. Hydrogen, being the lightest element highlights quantum effects more pronounced than the rest of the elements.In the case of non-crystalline or disordered materials, the models provide partial information and only a reduced sampling of possible configurations can be done at the present. With very large computing power, as exascale computing will provide, a new opportunity arises to study these systems and introduce a description of statistical configurations including energetics and dynamics characterization of configurational entropy. As part of the ICE-MAN project, we are developing the tools to manage the workflows, visualize and analyze the results. To use state of the art computational methods and most neutron scattering that using atomistic models for interpretation of experimental data

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