COMPUTER AIDED MOLECULAR DESIGN – A COARSE-GRAIN TOOL FOR ACCELERATING DISCOVERY OF MOLECULAR INTERACTIONS WITH CEMENT

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ABSTRACT

Computer aided (-assisted) molecular design (CAMD) involves all computer-assisted techniques used to discover, design and optimize compounds with desired structure and properties[1]. In this paper the use of CAMD is illustrated for the discovery of new shrinkage reducing admixtures (SRA's) and is framed as one of many multi-scale modeling tools in a broad toolkit of possibilities. The multi-scale modeling hierarch typically includes linkage of sub-models that make predictions of events that happen at nanometer to meter length-scales and at times that range from pecoseconds to some macroscopically observable time frame such as hours or days. The choice of length (and hence time) scales is dependent upon the phenomena to be predicted. The multi-scale modeling *toolkit* typically includes but is not limited to atomistic quantum mechanics, molecular dynamics, lattice-based techniques (e.g. Lattice Boltzmann Method (LBM), cellular automaton, etc.) and continuum mechanics. Where then does CAMD fit in, or does it? This paper endeavors to illustrate that indeed CAMD is a powerful coarse-grain tool in the multi-scale modeling hierarchy that can be used to quantitatively identify relationships between molecular structure and performance in targeted applications such as the design of admixtures for use in portland cement concrete.

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[1] IUPAC definition, see: http://goldbook.iupac.org/search.py?search_text=computer.