A Computational Molecular Technology for Complex Reaction Systems towards Innovative Materials: The Red Moon Approach

ABSTRACT:
For studying microscopically molecular aggregation systems, like cementitious materials, by molecular modeling, where chemical phenomena take place through complex reactions (CRs), the Red Moon (RM) approach, a new, efficient, and systematic RM methodology, plays a powerful computational tool. It was applied successfully for large-scale chemical reaction systems [1] to analyze several essential and valuable materials for next-generation industrial development [2, 3].
This talk will introduce the RM approach [1] with its application examples from a practical viewpoint [2, 3] and next propose and discuss a possible application work in the civil engineering field, especially for developing innovative cementitious materials.