A Computational Molecular Technology for Complex Chemical Reaction Systems: Red Moon Approach

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When we apply computational chemistry (CC) to diffusion and chemical reactions in "molecular aggregation states" where many atoms and molecules are gathering in condensation, such fact that these phenomena occur only very rarely has made it restrictive or sometimes impossible to treat them by first principles CC methods. Under the circumstances, we have recently developed Red Moon Method [1, 2], a new efficient and practical 'atomistic' simulation method combining Monte Carlo (MC) and molecular dynamics (MD) methods with a Rare Event-Driving Mechanism [1, 2]. It was applied successfully for large-scale chemical reaction systems [1, 2] to analyze several materials essential and valuable in next-generation industrial development [3, 4]. This talk will introduce the Red Moon approach with its application examples from a practical viewpoint [3, 4].

References

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