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上智大学 理工学部 物質生命理工学科 主催
理工学部・理工学振興会 共催

New computational chemistry methods for studying ionic liquids

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Accurate calculations of intermolecular interactions are important to the prediction of physicochemical properties of condensed systems such as ionic liquids. In this work a new modification of second-order Møller–Plesset (MP2) perturbation theory is proposed that allows us to predict intermolecular interactions for complexes consisting of both neutral and ionic species within chemical accuracy. The new method, termed the spin-ratio scaled MP2 (SRS-MP2) method, performs equally well for hydrogen bonded and dispersion-driven complexes.

学外の方の聴講歓迎・申込不要・参加無料

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