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Possibilities of the free-complement methodology for solving the Schrdinger equation of atoms and molecules

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Chemistry is a science of complex subjects that occupy this universe and biological world and that are composed of atoms and molecules. Its essence is diversity. However, surprisingly, whole of this science is governed by simple quantum principles like the Schrdinger and the Dirac equations. Therefore, if we can find a useful general method of solving these quantum principles under the fermionic and/or bosonic constraints accurately in a reasonable speed, we can replace somewhat empirical methodologies of this science with purely quantum theoretical and computational logics. This is the purpose of our series of studies – called exact theory in our laboratory. Some of our documents are cited below [1-8]. The key idea was expressed as the free complement (FC) theory (originally called ICI theory [3]) that was introduced to solve the Schrdinger and Dirac equations analytically. For extending this methodology to larger systems, order N methodologies are essential, but actually the antisymmetry constraints for electronic wave functions become big constraints. Recently [8], we have shown that the antisymmetry rule or 'dogma' can be very much relaxed when our subjects are large molecular systems. In this talk, I want to present our recent progress in our FC methodology. The purpose is to construct predictive quantum chemistry that is useful in chemical and physical researches and developments in institutes and industries. [1] H. Nakatsuji, Acc. Chem. Res. 45, 1480 (2012). [2] H. Nakatsuji and H. Nakashima, TSUBAME e-Science J. 11, 8, 24 (2014). [3] H. Nakatsuji, Phys. Rev. Lett. 93, 030403 (2004). [4] H. Nakatsuji and H. Nakashima, Phys. Rev. Lett. 95, 050407 (2005). [5] H. Nakatsuji, et al, Phys. Rev. Lett. 99, 240402 (2007). [6] H. Nakatsuji and H. Nakashima, J. Chem. Phys.142, 084117 (2015). [7] H. Nakashima and H. Nakatsuji, J. Chem. Phys. 139, 044112 (2013). [8] H. Nakatsuji and H. Nakashima, J. Chem. Phys. 142, 194101 (2015).