CHEMISTRY 4021/8021
MIDTERM EXAM — SPRING 2011

1. Molecular Mechanics and Semiempirical Molecular Orbital Theory (100 points)

We have read two papers this semester addressing the development of new parameters for a (semi)empirical model: Nicholas et al. presented zeolite force-field development and Anders et al. presented the extension of PM3 to include lithium. For this problem, compare and contrast parameter development in a molecular mechanics model vs. a semiempirical molecular orbital theory model. Thus, what similarities and differences are there in terms of numbers and kinds of parameters needed, means for determination/optimization of such parameters, kinds of validation data, etc.?

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2. Ab Initio Hartree-Fock (HF) and post-Hartree-Fock Theories (50 points)

a. Why must the HF self-consistent-field equations be solved iteratively?

b. What basis functions are there on a F atom and a H atom in the 6-31G(d) basis set?

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c.   Explain, ideally including any necessary equation(s), the following statement: An atomic orbital basis function is to a molecular orbital as a Slater determinant is to a configuration interaction (CI) wave function.

d.   What is spin contamination?