

Name: _____

CHEMISTRY 4021/8021
MIDTERM EXAM 2 — SPRING 2013

Q1) What is "dispersion"? How do different modeling techniques—both classical and quantum mechanical—include (or fail to include) dispersion? What kinds of "mistakes" would you expect to make in molecular modeling if your model fails accurately to account for dispersion? (30 points)

Q2) Four categories of density functionals include 1) LDA, 2) GGA, 3) meta-GGA, and 4) hybrid functionals. Explain how these categories differ from one another in terms of the "form" of their constituent functionals. Offer at least one example where a particular modeling problem might motivate a preference for a functional from one category more than from any of the others. (40 points)

Q3) The following two terms (written using atomic units) appear in the energy expression that would be computed for many functionals. Explain generally what the terms are and show that they do indeed each have the same (energy) units. (30 points)

$$\frac{1}{2} \iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 \qquad -\frac{9}{8} \left(\frac{3}{\pi}\right)^{1/3} \int \rho^{4/3}(\mathbf{r}) d\mathbf{r}$$

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OVERFLOW PAGE

use the backs of pages or p. 4 as needed