CHEMISTRY 4021/8021
MIDTERM EXAM 2 — SPRING 2014

Q1) What is self-interaction error and what role does it play in density functional theory?
(25 points)

use the backs of pages as needed

Q2) What advantages were there associated with using a pseudopotential on gold in the second problem set as opposed to an all-electron basis set? (25 points)
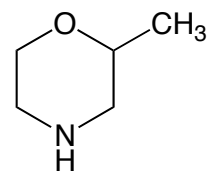
Q3) What is "dispersion"? How do different modeling techniques—both classical and quantum mechanical—include (or fail to include) dispersion? What kinds of "mistakes" would you expect to make in molecular modeling if your model fails accurately to account for dispersion? (25 points)

Q4) Discuss how one might go about computing the 298 K heat of formation ($\Delta H^{\mathrm{o}}_{f,298}$) of gaseous 2-methylmorpholine, focusing, obviously, on approaches covered in class (or the reading/videos) so far. Assign a level of confidence to the various protocols that you suggest, if not necessarily in quantitative terms, at least in a "best to worst" characterization. Note how computational constraints might play a role in limiting your range of choices, if at all. (25 points)