Benasque TDDFT - a DFT quiz

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I came across the following personality test in the back of a popular magazine. The questions are multiple-choice, and follow in the order of the lecture, more or less. You should circle correct answers as you identify them during the lecture. We will score the quizzes toward the end of the lectures, and there will be really great prizes for the top three students. So keep your pencils sharp.

1. Why are DFT calculations so much better than traditional methods?

   (a) You can do much larger systems.

   (b) They go much faster on the computer.

   (c) No-one can say for sure how accurate (or inaccurate) your calculation is.

   (d) All of the above.

2. Why are KS-DFT calculations typically much faster than traditional methods?

   (a) They yield really accurate densities

   (b) They only solve a non-interacting problem

   (c) They use perturbation theory

   (d) They use empirical information about the system

3. The Kohn-Sham kinetic energy is always

   (a) positive

   (b) negative

   (c) Sometimes one, sometimes the other

   (d) All of the above

4. The Hartree energy is always

   (a) positive

   (b) negative

   (c) Sometimes one, sometimes the other

   (d) All of the above

5. The exchange energy is always

   (a) positive

   (b) negative

   (c) Sometimes one, sometimes the other

   (d) All of the above

6. The correlation energy is always

   (a) positive

   (b) negative

   (c) Sometimes one, sometimes the other

   (d) All of the above

7. Which of the following would come out exactly right if evaluated on the Kohn-Sham wavefunction if you used the *exact* functional?

   (a) The kinetic energy

   (b) The one-body potential energy

   (c) The electron-electron repulsion energy

   (d) All of the above

8. The exact Kohn-Sham wavefunction and the true wavefunction for atoms are:

   (a) always equal

   (b) never equal

   (c) equal only for one-electron systems

   (d) different only for Fe

9. The density of the exact Kohn-Sham wavefunction and of the true wavefunction for atoms are:

   (a) always equal

   (b) never equal

   (c) equal only for hydrogen

   (d) different only for Fe

10. The Kohn-Sham wavefunction of density $n(\mathbf{r})$:

    (a) has density $n(\mathbf{r})$ and minimizes $\hat{T} + \hat{V}_{\text{ee}}$

    (b) has density $n(\mathbf{r})$ and minimizes $\hat{V}_{\text{ee}}$

    (c) has density $n(\mathbf{r})$ and minimizes $\hat{V}$

    (d) has density $n(\mathbf{r})$ and minimizes $\hat{T}$

11. Ground-state DFT can be used to calculate the gap of a bulk insulator

    (a) true

    (b) false

    (c) by correcting the KS gap

    (d) sometimes

12. Is DFT with approximate functionals empirical?

    (a) No, as long as you don't adjust the functional for your specific system

(b) No, even with functionals with a few empirical parameters

(c) No, as long as you stick with just one

(d) All of the above.

13. The magnitude of the total LDA exchange energy is:

(a) too small

(b) too big

(c) sometimes one, sometimes the other

(d) always exact

14. The magnitude of the total LDA correlation energy is:

(a) too small

(b) too big

(c) sometimes one, sometimes the other

(d) always exact

15. LDA overbinds molecules because the magnitude of total energies are:

(a) overestimated in LDA, and atoms are more uniform than molecules

(b) overestimated in LDA, and molecules are more uniform than atoms

(c) underestimated in LDA, and atoms are more uniform than molecules

(d) underestimated in LDA, and molecules are more uniform than atoms

16. DFT using LDA was not used for most chemical problems because:

(a) LDA calculations are unreliable

(b) LDA calculations are insufficiently accurate

(c) LDA calculations are too slow

(d) LDA calculations are too fast

17. The major improvement of GGA's over LDA is:

(a) Improved bond energies

(b) Improved bond lengths

(c) Improved electronic excitation energies

(d) Faster run times

18. Which functional will most closely satisfy the DFT Koopmans theorem, that $\epsilon_{HOMO} = -I$?

(a) LDA

(b) GGA

(c) EXX

(d) hybrid

19. The symmetry dilemma of stretched H_2 is that, when you do a standard DFT or HF calculation,

(a) you dont know what the correct spin state is

(b) you always get the wrong spin and wrong energy

(c) you either get the right spin and wrong energy, or vice versa

(d) you get the right spin and right energy, but for the wrong reasons

20. As I stretch H_2^+, the LDA self-interaction error

(a) will worsen

(b) becomes negligible

(c) will stay about the same

(d) is irrelevent