Name:

Reading HW

Submit your answers to Dr. Lan Li at the beginning of the class on Oct 3

Watch DFT Video – Intro to Computational Modeling and DFT Video 2 – Input Parameters for SIESTA Simulation, and read DFT Must-Remember Notes. Answer the following questions.

1. Briefly explain Schrödinger equation and Kohn-Sham method. (20 pts)

2. Briefly explain density functional theory. (20 pts)

3. Identify the statement below as true or false. And **provide a short explanation for your answer.** (10 pts each, 30 pts in total)

a. GGA for XC functional is more accurate than LDA.

b. More k points lead to a more accurate simulation, so we should use as many k points as possible in any simulation.

c. Basis set is a set of basic functions to describe wave function.

4. What parameters do you must specify to setup a SIESTA simulation? Briefly explain each of the parameters. (30 pts)

Important Note: Before Tuesday, Oct 3

If you don't have a nanoHUB account, please:

- Register at https://nanohub.org/register/
- Login to your account
- On "My Tools", select "MIT Atomic Scale Modeling Toolkit" as your "Favorites" tool.
- Launch "MIT Atomic Scale Modeling Toolkit"

If you have a nanoHUB account, please:

- Login to your account to make sure that your account remains active.
- Launch "MIT Atomic Scale Modeling Toolkit" on your dashboard.