CHUKA UNIVERSITY

UNIVERSITY EXAMINATIONS

EXAMINATION FOR THE AWARD OF DEGREE OF DOCTOR OF PHILOSOPHY IN CHEMISTRY

CHEM 902: PHYSICAL AND COMPUTATIONAL METHODS

STREAMS: PhD CHEMISTRY **TIME: 3 HOURS**

DAY/DATE: WEDNESDAY 18/12/2019 **2.30 P.M. – 5.30 P.M.**

INSTRUCTIONS:

- **This paper consists of FIVE questions.**
- **You are required to answer any FOUR questions out of FIVE.**
- **Do not write anything on this question paper.**

QUESTION ONE (15 MARKS)

Discuss the importance of finding solutions to the fundamental equation that describes the quantum behaviour of atoms and molecules, the schrödinger equation for scientific and technological progress.

QUESTION TWO (15 MARKS)

Outline the significance of the Bon-Oppenheimer approximation in the solution of the schrödinger equation, in settings of practical value.

QUESTION THREE (15 MARKS)

Outline the detailed information regarding the geometry that must be provided to a pre-compiled computer code in order to determine the electronic structure of the material.

QUESTION FOUR (15 MARKS)

Discuss the role of k points in determining the occupation of the electrons in the irreducible Brillouin zone of a unit cell.

QUESTION FIVE (15 MARKS)

Account in details for the information about the computational parameters required to stimulate the electronic structure of a material using a pre compiled simulation code.
