

## **Qualification Description**

**Subject Area: Computer chemistry**

**M. Sc. programme: Computational chemistry**

### **1. Educational objectives**

The programme offers theoretical training in the area of: quantum chemical methods for description of atoms, molecules, and periodic systems; structure-activity and structure-property relationships; molecular mechanics and molecular dynamics; rational molecular design; prediction and analysis of spectral characteristics; study of the mechanisms of chemical processes at the molecular level. The educational objective is achieved by courses focused on presenting in detail the major theoretical methods and on elucidating the structure-composition-properties relationship of chemical compounds.

### **2. Description**

The lectures of all courses are meant to provide theoretical training while the practical application will be mastered during the seminars by solving specific computational problems and/or performing molecular modelling within a particular chemistry-related assignment. The independent work of the students is stimulated – almost every course envisages individual student projects. The M.Sc. theses involve research on an up-to-date research topic and promote original scientific contributions.

### **3. Professional Qualifications**

Training of specialists with a definite profile at the Master EQF level in the field of Computational chemistry is provided. The graduates should acquire specific practical skills for performing analysis of numerical data from specialized software packages and for using various scientific programming languages to develop their own codes.

### **4. Professional Realization**

The graduate students with M.Sc. degree in Computer chemistry - Computational chemistry can continue their education in a related PhD programme or pursue successful career as researchers in computational modelling around the world. A business career is an equivalent option in industries like: ICT; pharmacy; biotechnologies; materials science; micro- and optoelectronics; photovoltaics; laser fabrication; ecology; nanotechnologies; catalysis, etc.

### **5. Admission requirements**

The candidates should hold B.Sc. degree in Chemistry or in a related area of study (certified by official Bulgarian translation of the diploma). They have to pass an admission exam in Chemistry.