	*Prof. Dr. Abdelilah Benyoussef* *Permanent member of the Hassan II Academy of Science and Technology, Founder of the former Laboratoire de Physique Statistique "now LaMCScI" , He is the coordinator of the poles of skills and knowledge on Condensed Matter, simulation and Modeling . editor in chief of the Moroccan Journal of Condensed Matter. He is President of the Moroccan Society of Statistical Physics and Condensed Matter. Abdelilah has a long-standing interest and expertise in Ab initio calculation and Monte-Carlo method of complex and new materials for renewable energy. His other fields of interest are Magnetism and phase transition in condensed matter; complex systems and critical self-organization in statistical physics. He is graduated from Paris-Sud University (1983). He is the founder of graduate program on statistical physics at the faculty of sciences Rabat, meanwhile he has trained several generations of graduate and undergraduate (bachelor degree) in the field of condensed material sciences and statistical physics*
Module	*Materials science and engineering*
Syllabus	*Material Energy Solutions: Computer Simulation & Modeling*
Courses description *Course objective* *Topics covered and Out of Class Assignments* 	*This syllabus is strongly recommended to students enrolled in physics, electrical engineering, materials science and chemistry. The courses cover state-of-the-art codes for the calculation of electronic, optical and magnetic properties to design novel materials with superior properties and functionalities. A dialogue between experimentalists and theoreticians to identify the most promising materials and devices related to energy, storage and sustainable environments. Density-functional theory (DFT) calculation are complemented by the molecular dynamics and the Monte Carlo simulations techniques to predict, explain, and control properties of materials at different scale. These courses focus on the study, by computer simulation and modeling, of nanomaterials studied in the syllabus "Nanomaterials from synthesis to energy applications". The great interest in different nanomaterials is motivated by the variety of properties they show, being candidates for numerous applications. Indeed, some nanomaterials are used for energy conversion using photovoltaic effect or as a metal-free water splitting (photo)catalyst. They are also used for energy storage; as in (Li/Na/Mg)-ion batteries or as solid state materials for hydrogen storage.* *Course objectives:* *•Understand how to build a model which describes the material to be simulated. The variables and the parameters describing the model are deduced from the calculations of the density functional theory of the ground state. In particular, crystalline structure, electronic structure, energy, stability and phase transitions. Thus, this course addresses the foundations of density functional theory and develops all the approximations and tools necessary for its implementation.* *• Understand how to do the detailed calculations of the electronic, magnetic, optical, electrical properties of the material in the ground state* *•Understand how to simulate the established model under the operating conditions (temperature, pressure, ...) of the material in the desired application. Particular emphasis is placed on materials for the conversion and storage of energy. This simulation makes it possible to calculate the properties (electronic, magnetic, electrical, optical, transport, etc.) of the material and thus predict its behavior under operating conditions even before manufacturing it. For the achievement of this objective, the Monte Carlo simulation is presented. Starting with the basics and going to the details of the parameterization and tools for its implementation for different applications.*
Pre-Requis	*Basic elements of quantum mechanics, Thermodynamics and statistical physics* *Basic elements of solid-state physics and material sciences* *Basic elements of Probability theory, numerical analysis and programming language.* *Basic elements of Non-equilibrium and dynamics*
Delivery & Duration	*Online Classes | #meeting per week, # hour each*
Who this programme is for	*Bachelor/Master/PhD*
Course Certificate of Completion	*Upon completion of a course, and once the participation has been verified, the candidate will receive an electronic certificate to download, print, and keep in his records* *Signed by the VLU/Prof. Abdelilah Benyoussef*
Technology Skill and Text book	*Typical Computer Science skills*
Textbooks, Sofwares, Codes	*Textbooks:* *Density Functional Theory: A Practical Introduction, David Sholl, Janice A Steckel* *Density Functional Theory in Quantum Chemistry, Takao Tsuneda* *Computational Materials Science : From Ab Initio to Monte Carlo Methods, Kaoru Ohno , Keivan Esfarjani, Yoshiyuki Kawazoe* *Monte Carlo Methods in Statistical Physics, M.E.J. Newman and G.T. Barkema* *Softwares: Fortran, C++,…, Codes: Wien2K, Quantun Espresso, Akai-KKR, ….*
Topics covered/Course Outline	*I- Density Functional Theory* *I-1 The foundation of modern density functional theory* *I-2 Kohn-Sham equations* *I-3 Density functional theory approximations* *I-4 Limits of density functionals* *I-5 analysis tools and Exchange-correlation hole* *I-6 Time-dependent DFT* *II- Monte Carlo simulation* *II-1 The principles of equilibrium thermal Monte Carlo simulation* *II-2 Simple sampling Monte Carlo methods* *II-3 Importance sampling Monte Carlo methods* *II-4 Systems with quenched randomness* *II-5 Sampling the free energy and entropy* *III- Nanomaterials for energy conversion and storage* *III-1 Graphene, the first truly 2D crystal* *III-2 Control of Graphene's Properties and applications* *III-3 Phosphorene* *III-4 Control of Phosphorene's Properties and applications (Photocatalytic hydrogen generation, hydrogen storage)*
Media Tools	*Online courses / Zoom management by Sabaek for Education & Training (Bahrain)*
Program Learning Outcomes (PLOs)	*The student will be able to* *(1)Select materials for photovoltaics application, Storage, or other specific applications.* *(2)Understand materials by properties targeting energy solution.* *(3)Use codes and solve standard problems and computations targeting materials performance for Solar cells, Li-batteries, membranes, Materials for chemical catalysis* *(4)Read scientific publications and technical documents dealing with the simulation and modeling* *(5)To discuss experiments results and analyse data critically/creatively and draw comprehensive conclusions*
Application Deadline	*Send an e-mail to info@vluplatform.net to receive zoom invitation*