Biomedical Technologies and Innovation Doctoral Programme (BIOTIN)

Title of the PhD Project	**Development of novel quantum-mechanical descriptors for nano-biomaterials and their application to predicting toxicity**
Acronym	**QMDESforNANO**
Research Fields of the Project	Nanotoxicology, Bioinformatics, Quantum Mechanics
Keywords	nanomaterials, predictive toxicology, machine learning, density functional theory
Host Institution, Department and Campus Location	Izmir Institute of Technology, Bioengineering Department, Urla/Izmir
PhD Awarding Institution and Graduate Programme	Izmir Institute of Technology, Graduate School, PhD in Bioengineering
Name and Affiliation of Main Supervisor	Asst. Prof. Ceyda Öksel Karakuş (IZTECH)
Name and Affiliation of Cosupervisors	Prof. Hasan Sahin (IZTECH) Assoc. Prof. Gokhan Karakulah (IBG)
Research Environment and Infrastructure	The selected candidate will have access to the research infrastructure available at Izmir Institute of Technology and Izmir Biomedicine and Genome Center. When a specific instrument or expertise is needed, all other national laboratories will also be contacted. http://safebionano.com/
Scientific Context of the Project	The rapid rise of nanotechnology has resulted in a parallel rise in the number of products containing nanomaterials. The unusual properties that nano forms of materials exhibit relative to the bulk has driven intense research interest and relatively rapid adoption by industry. Regulatory agencies are charged with protecting workers, the public, and the environment from any adverse effects of nanomaterials that may also arise because of these novel physical and chemical properties. They need data and models that allow them to flag nanomaterials that may be of concern, while balancing potential stifling of commercial innovation. Life sciences are progressively becoming more computational, relying on data-driven models to assist or replace experimental testing. Unlike bulk chemicals where we have large datasets to learn from, a major constraint hampering the development of models that can robustly predict nanomaterial properties and activity is the frequent lack of adequate descriptor data upon which to base estimates of model parameters.

	Computed theoretical descriptors that capture important structural properties of nanomaterials provide diverse sources of chemical properties and a broad coverage of the vast chemical property space describing all possible nanomaterials. Experimentally derived descriptors (e.g. size shape, solubility, agglomeration, etc) are of very limited use in machine learning models of biological effects of nanomaterials, not only because of their time and resource intensiveness, but also because they are not available for designed or otherwise hypothetical materials not yet synthesized. The core principle of machine learning in predictive toxicity domain is the expectation that structurally similar compounds will have similar biological activities. Molecular descriptors are commonly used in studies of molecular similarity to quantify the degree of structural overlap. However, almost all existing theoretical descriptors currently used are not nano-specific, meaning they are incapable of reliably discriminating between different-size forms of the same chemical substance. Development of novel descriptors that capture the specificity of nanoscale properties and the changes they undergo in different biological environments remains a challenging task, and will be an area of active research for some time.
Brief Workplan	The main aim of this thesis is to develop novel descriptors that can adequately express the size, time and environment-dependent properties of nanostructured materials that are commonly used in biomedical applications. The tentative yearly workplan is presented below: • **1st Year:** Training in machine learrning and data analytic tools, performing simple case studies with literature data • **2nd Year:** Training in quantum-mechanical calculations such as Density Functional Theory, developing novel theoretical descriptors for metallic nanoparticles • **3rd Year:** Application of both machine learning and quantum-mechanical approaches to experimental in-house nanotoxicity data, development of computational models that can predict the toxicity of nanoparticle-containing products
Innovative Aspects of the Project	The outcomes of the project will help develop innovative and feasible safer-by-design strategies for nanomaterials that are commonly used in biomedical applications and enable inherently safer design of advanced materials through structural manipulations. Thanks to the computational models developed using novel nanodescriptors, it will be possible to predict toxicity of nanomaterials at the design stage.
Training Opportunities of the Project	The selected candidate will be offered various training opportunities in the convergence of life sciences, material sciences and data science. The supervisory team and student will discuss and form a training plan at the start of the PhD, considering both personal interests and scientific needs.

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Interdisciplinary Aspects	The selected candidate will be supervised by three experts in nanotoxicology, quantum mechanics and bioinformatics. He/she will be working towards addressing multifaceted and multidisciplinary sub-topics that sit at the intersection of health, advanced materials and data science.
Intersectoral Mobility ☒ **Short Visit** ☐ **Secondment**	*Host:* Siemens Healthineers (TR) *Context of Mobility: Innovation management, Entrepreneurship, Prototyping, IP rights, 3D modelling*
Intersectoral Mobility ☒ **Short Visit** ☐ **Secondment**	*Host: Istanbul Health Industry Cluster (ISEK)* *Context of Mobility: Entrepreneurship Training, Thematic Pre-incubation Program*
International Academic Secondment	*Host Supervisor:* Prof. Francois M. PEETERS *Host Institution:* University of Antwerp, Antwerp, Belgium *Host Department:* Department of Physics *Duration:* 6 months *Estimated Time of Mobility: 2nd Year*
Main Supervisor	
Brief CV	**Asst. Prof. Ceyda OKSEL KARAKUS** **E-mail:** ceydaoksel@iyte.edu.tr **ACADEMIC DEGREES** Ph.D. Chemical Engineering University of Leeds, UK 2016 M.Sc. Chemical Engineering University of Leeds, UK 2012 Google Scholar: https://scholar.google.co.uk/citations?user=sdO-VFIAAAAJ&hl https://orcid.org/0000-0001-5282-4114
Co-supervisors	
Brief CV	**Prof. Hasan Şahin** **E-mail:** hasansahin@iyte.edu.tr **ACADEMIC DEGREES** Ph.D. Materials Science and Nanotachnology Bilkent University, Turkey 2014 Google Scholar: https://scholar.google.com.tr/citations?hl=tr&user=qwYs5WwAAAAJ https://orcid.org/0000-0002-6189-6707

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Brief CV	***Assoc. Prof. Gökhan Karakülah***

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ACADEMIC DEGREES

Ph.D.	Bioengineering	Dokuz Eylül University, Turkey	2014
M.Sc.	Medical Informatics	Dokuz Eylül University, Turkey	2009
B.Sc.	Biology	Ege University, Turkey	2005

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