DESIGNAÇÃO DO PROJETO | Qualidade e Segurança Alimentar — uma abordagem (nano)tecnológica

CÓDIGO DO PROJETO | NORTE-01-0145-FEDER-000011

OBJETIVO PRINCIPAL | The main research activities will be focused on mesoporous carbon nanoparticles (MCN) and amorphous carbon nanoparticles (CNP), as potential carriers of diagnostic markers and anti-cancer drugs (theranostics agents). The survey of modified (doped) graphene, as the primary material for the development of novel nanosensors for use in food safety and quality applications, will be also extensively investigated. Both activities will be rooted on accurate quantum-mechanical (QM) calculations of template carbon structures.

These calculations will then be used as the basis to develop accurate transferable force fields (FF), for the atomistic and coarse-grained (CG) modelling of MCN and CNP. Further QM calculations on the graphene-related template structures, including Ab-Initio Molecular Dynamics (AIMD) and Real-Time Time-Dependent Density Functional Theory (RTTDDFT), will be also performed. Finally, a systematic survey of the short and long-range effects of doped (nitrogen, oxygen, phosphorous and sulphur) atoms onto the graphene lattice will be carried. This will provide the basis for quantitative structure-properties relationships of graphene materials, with potential usefulness to design novel nanosensors for the food industry

ENTIDADE BENEFICIÁRIA| ICETA

DATA DE APROVAÇÃO: 01-04-2016 / **DATA DE INICIO:** 01-04-2016 / **DATA DE FIM:** 31-12-2019

INVESTIMENTO

CUSTO ELEGÍVEL APROVADO| 3 608 105,95 €

APOIO FINANCEIRO DA UNIÃO EUROPEIA |FEDER 85%

FUNDOS PRÓPRIOS |15%