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Interactive materials design towards a sustainable world

This talk will present recent contributions on computational materials discovery, ranging from carbon neutralization to energy transition [1-2]. Here, we have been inspired by the Sustainable Development Goals (SDGs) by the United Nations and the social role of Physics and Materials Science in developing technologies for a sustainable world. We apply a combination of data analytics and multiscale materials modeling to accelerate the materials discovery process and unveil the molecular mechanisms behind catalytic processes. Here, we focused on a multiscale approach, involving ab initio calculations, molecular dynamics, and machine learning for the development of new technologies for i) catalysts for direct conversion of CO2 to chemicals and fuel for carbon utilization, ii) in the processes of geochemical capture of CO2 through mineralization and clays, iii) gas separation, such as membranes, aiming at reducing CO2 emissions and flue gas separation [1-2], and iv) understanding of the fundamental processes in ethanol fuel cells. The fluid-material interactive design is also enhanced through perceptual experiences with interactive visualization techniques in virtual reality to design new materials and processes at multiple scales.

Keywords: Abstract; language; scientific articles; congresses.

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