



Dr. Parisa Nematollahi (Chemistry, BS, Tehran) got her master's degree in Inorganic Chemistry on wastewater purification with waste plants (2011, MS_c, Tehran). Due to her interest in Nanomaterials, she decided to study Nanochemistry (2016, MS_c, Tabriz) where she changed her research method from experimental to computational investigations. Her research activity focused on gas conversion reaction mechanisms on single metal atom doped graphene and graphene-like nanocatalysts using density functional theory (DFT) calculations.

She joined the PLASMANT group in January 2017 and worked on the computational design of heterogeneous nanocatalysts for methane and CO₂ conversion. Moreover, to understand the kinetics of the gas conversion reactions on the modified nanocatalysts she has developed a microkinetic model for the used systems (2020, Ph.D. Antwerp). In 2020 she awarded by the national research foundation (FWO, Belgium). Her current postdoc project is the computational exploration of new pathways in gas conversion on novel nanocatalysts.