POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 41st cycle

THEMATIC Research Field: ADVANCED CHARACTERIZATION OF SINGLE-ATOM CATALYSTS

Monthly net income of PhDscholarship (max 36 months)
1500.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	Single-atom catalysts (SACs) hold promise in revolutionizing heterogeneous catalysis, due to their unparalleled efficiency and selectivity and maximized metal utilization. However, elucidating the intricate mechanisms governing the performance of single-atom catalysts in liquid-phase reactions remains a formidable challenge. This Ph.D. project aims to design SACs that enable environmentally friendly and energy-efficient chemical reactions, reducing the dependency on rare and expensive metals, minimizing waste production, and improving reaction efficiencies.
Methods and techniques that will be developed and used to carry out the research	To achieve these objectives, the research will employ a multidisciplinary experimental approach. Synthesis techniques such as atomic layer deposition (ALD) will be used to precisely control the deposition of single atoms on various support materials, while wet chemistry methods, including impregnation and colloidal synthesis, will prepare nanostructured supports and deposit single atoms. Characterization methods, including transmission electron microscopy (TEM), X-ray absorption spectroscopy (XAS), X-ray photoelectron spectroscopy (XPS), and scanning tunneling microscopy (STM), will provide high-resolution imaging and analysis of single

	atoms, their local electronic and structural environment, and their chemical states and surface composition. Catalytic testing will involve reactor studies to evaluate activity, selectivity, and stability under various conditions, kinetic studies to understand reaction mechanisms and determine rate-determining steps, and in-situ and operando techniques to monitor catalytic processes in real-time under actual reaction conditions. Integration and scale-up efforts will include pilot-scale reactors to test the scalability and industrial applicability of the developed SACs and techno-economic analysis to evaluate the cost-effectiveness and commercial potential of the new catalytic processes.
Educational objectives	This research will provide a comprehensive training platform encompassing theoretical knowledge, experimental skills, and computational techniques. Through hands-on experience with advanced instrumentation and interdisciplinary collaboration, the PhD candidate will develop proficiency in advanced characterization methods, data analysis, and scientific communication, fostering critical thinking and problem-solving abilities essential for tackling complex scientific challenges.It is expected that the PhD candidate will publish multiple highly-cited papers in prestigious journals such as *Angewandte Chemie International Edition*, *Journal of the American Chemical Society*, *Nature Catalysis*, *Nature Materials*, and *Nature Synthesis*. Furthermore, the PhD candidate will actively present their work through several oral talks at prominent conferences such as the European Congress on Catalysis, North American Meeting, and other scientific gatherings.
Job opportunities	Graduates of this Ph.D. program will be highly sought after in both academia and industry. Opportunities abound in research institutions, national laboratories, and industrial R&D sectors, where their specialized skill set, and innovative mindset will be instrumental in driving forward the development of next-generation catalysts and sustainable chemical processes.
Composition of the research group	0 Full Professors 1 Associated Professors

	5 Assistant Professors 7 PhD Students
Name of the research directors	Prof. Gianvito Vilé

Contacts
Telephone: +39 02 2399 3036 E-mail: gianvito.vile@polimi.it Webpage: https://www.vile-researchgroup.com/

Additional support - Financial aid per PhD student per year (gross amount)			
	1st year	**2nd year**	**3rd year**
Housing - Foreign Students	2000.0 € per student	2000.0 € per student	2000.0 € per student
	max number of financial aid available: 1, given in order of merit ..		
Housing - Out-of-town residents	--		

Scholarship Increase for a period abroad	
Amount monthly	750.0 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Individual budget for research (about 6.000 euro): 1st year: about 2.000 euro; 2nd year: about 2.000 euro; 3rd year: about 2.000 euro **Teaching assistantship** (availability of funding in recognition of supporting teaching activities by the PhD student): there are various forms of financial for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.