POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 39th cycle

THEMATIC Research Field: MECHANISMS OF AROMATIC PYROLYSIS AND OXIDATION

Monthly net income of PhDscholarship (max 36 months)
€ 1400.0 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	Titolo: Biomass gasification for hydrogen production Acronimo: Bio4H2 CUP: D53D23003140006 Codice Progetto: 20227W5CLJ Decreto di Concessione: D.D. ammissione finanziamento PE8 prot.961.30-06-2023 Gasification of solids has recently emerged as an interesting approach among the portfolio of technologies that are currently being developed as viable pathways towards the transition to an environmentally sustainable and fully decarbonized energy sector. Despite the possibilities offered by the gasification technology, the number of working gasifiers is quite small, often at the pilot scale, and troubled by many operational difficulties. The difficult implementation of gasification can be directly related to the lack of knowledge of the process. The aim of this project is to shed a light on one specific key aspect of gasification: its kinetics.
Methods and techniques that will be developed and used to carry out the research	Ab.initio quantum chemistry methods will be used to investigate fundamental reactions of interactions between oxygenated species (like O2, OH ,O) and aromatic structures in the gas phase and extended to surface reactions between similar functionalities. Similarly, the same theoretical approach will be used to investigate the

	competing pyrolysis pathways, investigating aromatic interactions resulting in the formation of larger Polycyclic Aromatic Hydrocarbons.
Educational objectives	The educational objectives are to allow the PhD student to learn the modeling of complex reacting systems and use this expertise to design more robust and optimized gasifiers.
Job opportunities	This activity will open several job opportunities in the field of renewable energies especially in engineering companies. Above all, understanding fundamentals of reaction mechanisms will offer many opportunities in R&D departments and research centers.
Composition of the research group	2 Full Professors 2 Associated Professors 3 Assistant Professors 10 PhD Students
Name of the research directors	Prof. Tiziano Faravelli

Contacts
Telephone: +39 02 2399 3282 Email: tiziano.faravelli@polimi.it Web-pages of the research group: http://creckmodeling.chem.polimi.it/

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	700.0 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Educational activities (funding for participation in courses, summer schools, workshops and conferences) - financial aid per PhD student per year: 1st year: around 1.900 euros per student 2nd year: around 1.900 euros per student 3rd year: around 1.900 euros per student

Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student:
There are various forms of financial of 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.