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PUBLIC SELECTION FOR RECRUITING NO. 1 FIXED-TERM RESEARCHER, ART. 24, PARAGRAPH 3, LETTER A) OF ITALIAN LAW NO. 240/2010, IN ACADEMIC RECRUITMENT FIELD 03/A2 - MODELS AND METHODS FOR CHEMISTRY AND ACADEMIC DISCIPLINE CHIM/02 - PHYSICAL CHEMISTRY *FOR THE DEPARTMENT OF SCIENCE AND TECHNOLOGICAL INNOVATION* ***(CODICE BANDO 2024-RTDA_CHIM/02_PRIN_PNRR)***

DEPARTMENT	DEPARTMENT SCIENCE AND TECHNOLOGICAL INNOVATION
PLACE OF EMPLOYMENT	ALESSANDRIA
ACADEMIC RECRUITMENT FIELD	03/A2 - MODELS AND METHODS FOR CHEMISTRY
ACADEMIC DISCIPLINE	CHIM/02 - PHYSICAL CHEMISTRY
ELIGIBILITY REQUIREMENTS (MANDATORY)	PhD or an equivalent academic title, based on international treaty agreements and the applicable norms
RESEARCH ACTIVITIES	The required profile corresponds to a Chemist-Physicist or a Theoretical Physicist of Matter with solid theoretical and computational skills, who can integrate into the general activity of the field with special emphasis on project-related activities: (i) PRIN2022 2022WS44W4 "EnvELOP" responsible Dr. Ciro A. Guido; (ii) PNRR M2C2 "Ecostore-H2" responsible Prof. Leonardo Marchese. The main focus of the "EnvELOP" project is the development of new theoretical-computational methodologies for the multiscale description of the photophysics and photochemistry of complex molecular systems, with particular attention to the accurate simulation of the interactions between a molecular system and the external environment. The "Ecostore-H2" project is mainly aimed at the design, synthesis and characterization of new materials for energy, gas adsorption and "green chemistry": the modeling activity at DISIT will flank and support the experimental work as well as must contribute to the development of integrated (theoretical/experimental) investigation techniques. The new professional will use the most advanced theoretical and computational techniques as an integral and indispensable part of the design and characterization of new molecular systems. The main areas of activity, for which specific high-level skills are required, are: a) quantum calculations at the molecular level, using DFT and post-Hartree-Fock techniques, with explicit consideration of contributions due to the environment in which the system is located, for the description of structures, energies, electronic properties, and

	reactivity in model systems; b) proven experience in theoretical development and implementation in computational codes of QM/classical methods for the description of molecular excited states in the presence of an external environment (solvent, metal nanoparticles and protein matrices or materials); c) Classical Molecular Dynamics simulations aimed at describing. Large complex systems, including in mixed approaches QM/MM.
SCIENTIFIC TARGETS	The activity of the new staff unit should integrate into the research of the group belonging to the CHIM/02 Sector, leading to scientific publications, at least 1 per year, and participation in national or international conferences, at least 1 per year.
REQUESTED TEACHING DUTIES	The new staff unit is expected to carry out teaching assignments integrative up to 3 CFU/year for the Theoretical and Computational Chemistry courses of the Master's Degree in Chemical Sciences, and of a seminar nature for the doctoral school in "Chemistry and Biology" relevant to S.S.D. CHIM/02 PHYSICAL CHEMISTRY.
LANGUAGE	English and Italian
NUMBER OF SELECTED PUBLICATIONS REQUIRED	15