Annex A – Positions with specific topic

Ph.D. Course	**METHODS AND MODELS FOR MOLECULAR SCIENCES**
Scholarship type	MISSIONE 4 – ISTRUZIONE E RICERCA Investimento 4.1 - Dottorati di ricerca PNRR (art. 8, DM 118/2023)
N.	2
CUP	**E53C23001320001**
Title	**1) Computational design of new materials for applications in the field of renewable energy sources** **2) Computational strategies for the simulation of the atmospheric reactivity of molecular species in the gaseous phase**
Brief description of the research project	1) The scholarship will mainly be aimed at forming a profile of a scholar capable of tackling the study of complex chemical systems, which can potentially be used in the design of new materials for use in the field of renewable and low environmental impact energies. The scholar will use state-of-the-art techniques based on hybrid multiscale/multilevel computational models as well as mechanical/classical ones also in combination with molecular dynamics. 2) The scholarship will mainly be aimed at forming a profile of a scholar capable of tackling issues related to climate change with the theoretical and methodological tools of computational chemistry. The scholar will employ state-of-the-art quantum computational techniques and protocols to understand the degradation mechanism of air pollutants and the related chemical kinetics in order to evaluate their life time and understand their potential environmental impact.
SSD	CHIM/02, CHIM/12
Period of study and research to be carried out abroad	It is mandatory to carry out periods of study and research in companies or research centers from a minimum of six (6) months to a maximum of twelve (12) months, even if not continuous, and periods of study and research abroad, The destinations for each student will be decided by supervisors and the Ph.D course board.