class	PI name	PI surname	institution	project title	BUDGET
A	Marco	BERNASCONI	University of Milano-Bicocca	Simulation of GeTe nanowires for phase change memories	900.000
A	Stefano	DE GIRONCOLI	SISSA and CNR-IOM DEMOCRITOS	Determination of cholesterol crystal structure in human gallstones from first-principles	1.000.000
A	Marco	DE VIVO	Italian Institute of Technology	Enhanced sampling simulations to investigate the catalytic metal binding site of Type II topoisomerases	1.000.000
A	Stefano	FABRIS	CNR-IOM DEMOCRITOS	Functionalized carbon nanotubes for artificial photosynthesis	800.000
A	Francesco	FILIPPONE	Consiglio Nazionale delle Ricerche	Properties of interfaces in ternary hybrid materials for photovoltaic applications.	800.000
A	Alfonso	GAUTIERI	Politecnico di Milano	Molecular dynamics based investigation of Microscale and Mesoscale Mechanisms of Osteogenesis Imperfecta	819.200
A	Marco	MASIA	Universita' degli Studi di Sassari	Theoretical Insights of CO2 Storage and Separation in Zeolite Imidazolate Frameworks with Ab initio Molecular Dynamics Simulations	700.000
A	Carlo	PIERLEONI	L'Aquila	Coupled Electron-Ion Monte Carlo Study of High Pressure Hydrogen	640.000
A	Giulio	RASTELLI	University of Modena and Reggio Emilia	Binding Estimation After Refinement, a powerful tool for virtual screening of potential drugs	500.000
A	Silvano	SIMULA	INFN - Sezione Roma Tre	A New Approach to B-Physics on Current Lattices	560.000
A	Paolo	UMARI	CNR-IOM	Many-body effects on the electronic structure of DNA and of its oxidative damage	1.000.000
B	Vincenzo	ARMENIO	università degli studi di Trieste	Large Eddy Simulation of neutral and strongly stratified flow on a diffuser with a free surface	70.000
B	Valerio	BELLINI	CNR	Switching and Anchoring Molecular Magnets on Surfaces	80.000
B	Enrico	BODO	Sapienza, University of Rome	Atomistic Simulation of Ionic Liquids: Theoretical studies of Their Local Nanoscopic Structure.	38.400
B	Stefano	BORGANI	University of Trieste	Cosmological Simulations of a Large Sample of Massive Galaxy Clusters: The effect of the Black-Hole Feedback	100.000
B	Dario	BORGOGNO	Politecnico di Torino	Electron dynamics in 3D collisionless magnetic reconnection	150.000
B	Fabrizio	BRIGHENTI	Universita' di Bologna	3D hydrodynamical simulations of AGN feedback in galaxy clusters, groups and galaxies	120.000
B	Massimo	CAPONE	CNR-IOM and SISSA	Magnetism in Correlated Materials: from exotic superconductors to functional oxides	150.000
B	Sergio	CARACCIOLO	Universita' degli Studi di Milano, Dip di Fisica	Phase transitions and computational hardness in constraint satisfaction problems	150.000
B	Letizia	CHIODO	Italian Institute of Technology - IIT	excited state properties of TItanium DIoxide hybrid surfaces: Photocatalysis and pHOtovoltaics throught ab initio many body Methods.	142.000
B	Giancarlo	CICERO	Politecnico di Torino	An ab initio study of pure and tin doped amorphous and crystalline In2O3	100.000
B	Gabriele	D'AVINO	Bologna University	Simulation of fullerene/sexi-thiophene interfaces for organic photovoltaics applications	140.000
B	Lucilla	DE ARCANGELIS	Second University of Naples	Structural and mechanical properties of hydrogels	122.880
B	Alessandro	DE VITA	Trieste	CITRATE ON GOLD: AN EXPERIMENTAL AND THEORETICAL APPROACH TO BIOSCIENCE	150.000
B	Rossella	FERRETTI	University of L'Aquila	Investigating convection in the Mediterranena area: role of the resolution using LES	76.800
B	Ettore	FOIS	Universita' degli Studi dell'Insubria	CO on Nanosized Titania: Unravelling strong Lewis acid sites at anatase (TiO2) surfaces.	120.000
B	Alessandra	FORNI	CNR-ISTM	Development of a computational approach to describe halogen bonding in biological macromolecules	90.000
B	Giuseppe	FORTE	Università di catania	Simulations of the Structural, Optical and Electronic Properties of Graphene	20.000
B	Simone	FURINI	University of Siena	Molecular Dynamics simulations of repressor proteins scanning the DNA sequence	140.000
B	Antonio	GHIDONI	Università degli studi di Brescia	High-order Accurate discontiNuous Galerkin sOlUtion of Turbulent flows	140.000
B	Gianluca	GIORGI	University of Siena	Gas phase studies of properties and reactivity of bioorganic ions	90.000
B	Paola	GORI	CNR	Electronic and optical Properties of functionalized group IV 2D HExagonal Structures	100.000
B	Claudio	GRECO	Università Milano-Bicocca	Protons and electrons transfer towards [FeFe]-hydrogenases active site models: fundamental hints for H2 evolution catalysis	80.000
B	Massimiliano	GUARRASI	Universita' degli Studi di Palermo	Modelling of Heating of COronal Loops	120.000
B	Andrea	IENCO	ICCOM-CNR	Computational Studies on Metal Cluster Chemistry. Part 2	100.000
B	Antonio	LAGANÀ	University of Perugia	COUPLING HIGH PERFORMANCE WITH HIGH THROUGHPUT CALCULATIONS TO STUDY THE N2 + N2 REACTION	90.000
B	Maria Paola	LOMBARDO	INFN	Numerical analysis of the phases of strongly coupled gauge theories, and the chiral boundary of QCD	100.000
B	Alessandra	MAGISTRATO	CNR-IOM-Democritos	Structure and function of the human aromatase investigated by molecular simulations.	129.000
B	Ivan	MARRI	Universita' degli Studi di Modena e Reggio Emilia	ab-initio Study of the OpticaL and Electronic properties of dye-sensitized NANOstructures	149.000
B	Lorenzo	MASCHIO	Università degli Studi di Torino	Post Hartree-Fock computational study of the Interaction of Molecules in microporous Metal-Organic Frameworks	150.000

B	Andrea	MIGNONE	Torino	Current-Driven Instabilities in Three Dimensional Relativisitc Jets	140.000
B	Susanna	MONTI	National Research Council (CNR)	Investigation of the dynamics and adsorption characteristics of nucleic acid structures on titania surfaces.	80.000
B	Giuseppe	MURANTE	INAF- Osservatorio Astronomico di Torino	Galaxy formation simulations with an innovative sub-grid model for star formation and feedback in presence of chemical enrichment and metal cooling	105.000
B	Stefano	OSSICINI	Universita' degli Studi di Modena e Reggio Emilia	Auger Recombination and Carrier mUltiplication in Si-nanostructures	136.000
B	Daniele	PALA	University of Parma	Influence of cholesterol on the stability of G-protein coupled receptors assessed by long-timescale MD simulations	150.000
B	Francesco	PEDERIVA	University of Trento - Physics Department	Theory of HYpernuclei by Quantum Monte Carlo Methods	100.000
B	Carlo	PETRONGOLO	University	Non-adiabatic dynamics and simulation of atom+diatom collisions	150.000
B	Deborah	PREZZI	CNR - Nanoscience Institute	Coupling with graphene through Cu and metal adlayers	90.000
B	Sabrina	PRICL	University of Trieste	Designing new nanovectors for RNA therapeutics using computational and experimental methods	150.000
B	Olivia	PULCI	University of Rome Tor Vergata, and ETSF	Step induced Anisotropy in the optical properties of Diamond	120.000
B	Chiara	ROMUALDI	University of Padova	A computational approach using the integration of gene expression and pathway topology for the reconstruction of biological networks	100.000
B	Giacomo	ROTOLI	SUN - Seconda Università di Napoli	Noise and Dissipation in Josephson junction quantum based systems.	80.000
B	Jacopo	SGRIGNANI	CNR-IOM-Democritos (SISSA/ISAS)	Molecular Recognition Mechanism of DNA Damages Investigated via Molecular Simulations: The prototypical case of Uracil DNA Glycosylase.	119.000
B	Domenico	SUMMA	Universita' di Bologna	The MEsophases of the alpha,omega-bis(4'cyanobiphenyl-4-yl) undecane symmetric diMER (11BCB)	141.176
B	Francesco	TARANTELLI	Università di Perugia	Au(I)-based molecular catalysts: from know-how to know-why	150.000
B	Federico	TOTTI	Univeristy of Florence	The {FeIII4} SMM grafted on Au(111):Exploring PES for an optimum candidate	150.000
B	Francesco	ZONTA	Universita' degli Studi di Padova	MOLECULAR DYNAMICS OF HEMICHANNELS FORMED BY CONNEXIN PROTEIN SUBUNITS: A THEORETICAL APPROACH TO CONNEXIN STRUCTURE, FUNCTION AND DYSFUNCTION	100.000