

class	PI name	PI surname	institution	project title	BUDGET	hpc system
A	Andrea	BENAZZO	Università di Ferrara	Temporal sampling scheme and demographic inferences in population genetics	600.000	PLX
A	Guido	BOFFETTA	University of Torino	Double Diffusive Turbulence	200.000	IBMPower6,
A	Ezio	BRUNO	University of Messina	Ab initio study of phase transitions in metallic alloys: equilibrium thermodynamics and kinetics	350.000	PGP
A	Francesco	CALIFANO	University of Pisa	Non linear 3D plasma dynamics in a magnetized plasma driven by shear flows instabilities	600.000	IBMPower6,
A	Francesca	FANELLI	University of Modena and Reggio Emilia	High-Throughput Virtual Screening of Inhibitors of RhoA-Lbc Interaction	200.000	BGP
A	Pasquale	LONDRILLO	inaf bologna	PIC Numerical Investigation of plasma based electron acceleration	300.000	BGP
A	Massimo	OLIVUCCI	Università di Siena	Computational Engineering and Prediction of Excited State Properties of Bacterial Photoreceptor Mutants	200.000	IBMPower6,
A	Salvatore	ORLANDO	Istituto Nazionale di Astrofisica	Mass accretion onto young stellar objects driven by flaring activity in protostellar disks	450.000	IBMPower6,
A	Sergio	PIROZZOLI	Universita' di Roma 'La Sapienza'	Large scale direct numerical simulation of Supersonic TURbulent Boundary layers at high Reynolds number	1.000.000	BGP
A	Federico	PISCAGLIA	Politecnico di Milano	Large-eddy simulation on unstructured meshes for internal combustion engines	600.000	PLX
A	Mauro	SBRAGAGLIA	University of Rome Tor Vergata	Advanced numerical simulations of non ideal multicomponent turbulent convection	614.000	IBMPower6,
A	Alessandro	STROPPIA	CNR-SPIN	Ab-initio study of new Multiferoic Metal-Organic Frameworks (MOFs)	1.200.000	IBMPower6,
A	Federico	TOTTI	Univeristy of Florence	A step forward to future devices: DFT simulations of SMM on Manganites.	700.000	IBMPower6,
A	Attilio	VARGIU	Istituto Officina dei Materiali (IOM) (CNR), Unita' Operativa SLACS	Molecular Description of Efflux Dynamics in Gram-negative Bacteria: an Extensive Study on Antibiotics and Inhibitors of E.Coli and P.Aeruginosa RND pumps	872.448	IBMPower6,
B	Michele	AMATO	Universita' di Modena e Reggio Emilia	Semiconductor Nanowires for Photovoltaics: Ab-initio Description of Doping at Nanoscale	146.880	IBMPower6,
B	Giovanni	BARCARO	Consiglio Nazionale delle Ricerche (CNR)	Highlighting Order in Metal NanoAlloys	150.000	IBMPower6,
B	Paola	BELANZONI	Universita' degli Studi di Perugia,	Device oriented applications of non-isovalent alloys: from photovoltaics to water splitting	70.000	IBMPower6,
B	Valerio	BELLINI	CNR	Cr Heterometallic Rings On Metals	100.000	IBMPower6,
B	Luca	BELLUCCI	Center S3, CNR-INFN Institute of Nanoscience	Probing conformations of peptides at gold/water interface: the first step to study how metal surfaces affect the protein folding.	150.000	IBMPower6,
B	Enrico	BENASSI	Centro S3, CNR Istituto di Nanoscienze	Azo-benzene derivatives in solution and on surfaces: Optical and Mechanical Properties	100.000	IBMPower6,
B	Stefano	BORGANI	University of Trieste	Feedback effects on the large-scale distribution of cosmic baryons	125.000	IBMPower6,
B	Giorgia	BRANCOLINI	CNR-NANO, Institute of Nanoscience	Modeling Proteins interactions with Solid Nanoparticles	140.000	IBMPower6,
B	Fabrizio	BRIGHENTI	Università di Bologna	High resolution 3D hydrodynamical simulations of AGN feedback in elliptical galaxies	150.000	IBMPower6,
B	Silvia	CASASSA	University of Turin	Dispersive Interaction deciding the relative stability of Al ₂ SiO ₅ Orthosilicates and Al Hydroxides.	150.000	IBMPower6,
B	Alessandra	CATELLANI	CNR-IMEM	Functionalization of SiC surfaces & wires	130.000	IBMPower6,
B	Carlo	CAVALLOTTI	Politecnico di Milano	Molecular modeling of Agar-Carbomer Hydrogels in 3 dimensions	150.000	IBMPower6,

B	Matteo	CECCARELLI	University of Cagliari	Structure to function relationship of ancestral globin proteins	150.000	IBMPower6,
B	Letizia	CHIODO	Italian Institute of Technology	Unraveling the role of oxygen vacancies and interstitial Ti atoms on the optical properties of TiO2 crystals with MBPT approaches	129.570	IBMPower6,
B	Francesco	COLIZZI	SISSA	Step-by-step RNA unwinding	100.000	IBMPower6,
B	Piero	DECLEVA	University of Trieste	Chirality in Photoemission	150.000	IBMPower6,
B	Elena	DEGOLI	Universita' di Modena e Reggio Emilia	Non Stoichiometric lead chalcogenides Nanocrystals for photovoltaics by first principles	75.000	IBMPower6,
B	Alessia	DI VITO	University of Rome Tor Vergata	Study of the influence of surface steps on the optical anisotropy of the Au(110) surface	120.000	IBMPower6,
B	Nicola Luigi	DURANTE	CNR	The optical properties of metal alloy nanoclusters	150.000	IBMPower6,
B	Alessandra	FORNI	CNR-ISTM	Highly efficient organic and coordination chromophores for applications in visible and NIR photoluminescence and in non linear optics	125.000	IBMPower6,
B	Cosimo Gianluca	FORTUNA	University of Catania	Simulations of new trans-HeteroArylEthenes as NLO and photovoltaic lead compounds	40.000	IBMPower6,
B	Ignazio	FRAGALÀ	University of Catania	molecular systems on metal oxide surfaces. Adsorption process and catalytic properties	90.000	PLX
B	Viviana	GARBUIO	Tor Vergata university, Rome	Disorder effect on the excited state properties of the hexagonal ice surface	100.000	IBMPower6,
B	Alfonso	GAUTIERI	Politecnico di Milano	In silico Mechanical Investigation of Chondroitin Sulphate	153.600	IBMPower6,
B	Tahereh	GHANE	Universita' di Modena e Reggio E.	Dynamical effects in the optical absorption of DNA triplexes	123.000	IBMPower6,
B	Franco	GIANTURCO	Sapienza University of Rome	Quantum molecular dynamics in the interstellar medium	50.000	IBMPower6,
B	Guido	GOLDONI	University of Modena	Optical properties of metallo-organic chromophores in different dielectric environments for photovoltaic applications	108.864	IBMPower6,
B	Paola	GORI	CNR	Silicon on Ag (110) and (111): structure, Electronics and optical properties	150.000	IBMPower6,
B	Marco	GOVONI	Universita' degli Studi di Modena e Reggio Emilia	Multiple Exciton Generation in Si nanostructures for photovoltaic applications	150.000	IBMPower6,
B	Roberto	GUERRA	Universita' di Modena e Reggio Emilia	Enhanced Conductivity In Photovoltaic Solar Cells: The Silicon Nitride Alternative	140.000	IBMPower6,
B	Leonardo	GUIDONI	Universita' de L'Aquila	The Bond-Length Alternation of polyacetylene chains by Quantum Monte Carlo	150.000	IBMPower6,
B	Johon	HELLSVIK	CNR-SPIN	Magnetic Order By Disorder in Cupric oxide	20.000	IBMPower6,
B	Conor	HOGAN	CNR-ISM and ETSF	Simulating spectroscopy at complex surfaces	111.000	SP6 + BGP
B	Carmelo	LA ROSA	University of Catania	Theoretical approach to the interaction of resveratrol and its derivatives with Islet Amyloid Polypeptide (IAPP): anti-aggregation capability of small molecules through Molecular Dynamics calculation.	72.800	IBMPower6,
B	Giuseppe	LANZA	Università di Catania	Quantum-chemical approach to energetic and structure of norbornene/norbornano amino acid based peptides	20.000	IBMPower6,
B	Andrea	LOMBARDI	Università di Perugia	Molecular collisions and energy transfer in atmospheric chemistry and gas dynamics	100.000	IBMPower6,
B	Maria Paola	LOMBARDO	INFN LNF (on leave to Humboldt Universitaet zu Berlin)	Numerical analysis of the phases of strongly coupled gauge theories II : the chiral boundary, and exploratory studies of the conformal dynamics	150.000	IBMPower6,
B	Alessandra	MAGISTRATO	CNR-IOM-Democritos	Molecular modeling of Human Aromatase in its biological environment and characterization of the access/release pathways from/to the catalytic site.	169.000	IBMPower6,
B	Rita	MAGRI	University of Modena and Reggio Emilia	Semiconductor Nanowire Design for Advance Device Applications	74.000	IBMPower6,
B	Layla	MARTIN-SAMOS	CNR-IOM	OPTical signature of point defects in silica based FIBERS	148.000	IBMPower6,

B	Lars	MATTHES	University of Rome Tor Vergata	Electronic and optical properties of Cu/Ag/Cu clusters on carbon nanotubes	150.000	IBMPower6,
B	Simone	MELCHIONNA	Consiglio Nazionale delle Ricerche	Inquiring protein thermo-stability	150.000	SP6(BGP)
B	Emiliano	MERLIN	University of Padova	The Magellanic Clouds: hypothesis of formation and evolution. A numerical study	120.000	IBMPower6,
B	Michele	MIGLIORE	CNR	Neuronal computations: from cognition to neuropathologies 2	150.000	IBMPower6,
B	Franco	MOGLIE	Universita' Politecnica delle Marche	Optimization of electromagnetic reverberation chambers using FDTD simulations	115.000	SP6 + BGP
B	Pierluigi	MONACO	Universita' di Trieste	Radiative cooling in galaxy formation: a numerical benchmark test for galaxy formation models	144.300	IBMPower6,
B	Adriano	MOSCA CONTE	University of Rome Tor Vergata	Understanding the yellowing of ancient paper	120.000	IBMPower6,
B	Miguel	ONORATO	Universita' di Torino	NUMERICAL SIMULATIONS OF THE GROSS-PITAEVSKII EQUATION IN 2 AND 3 DIMENSIONS: CONDENSATION AND KELVIN WAVES	100.000	PLX
B	Stefano	OSSICINI	Universita' di Modena e Reggio Emilia	Ternary semiconductor NANOparticles for SOLar cElls	75.000	IBMPower6,
B	Maria	PERESSI	Universita' di Trieste	NiCu: a strategic alloy model catalyst for organic synthesis	150.000	IBMPower6,
B	Denise	PERRONE	Universita' della Calabria	Alpha particles influence in Solar Wind alfvénic TURBulence	150.000	IBMPower6,
B	Simone	PICCININ	CNR-IOM DEMOCRITOS	The Role of Sub-surface Oxygen in Ethylene Epoxidation on Ag-Cu alloys	165.888	IBMPower6,
B	Evgeny	PLEKHANOV	Dipartimento di Fisica	Mott Physics via 3d/4d Substitution in Transition Metal Oxides	153.600	IBMPower6,
B	Piero	PROCACCI	Firenze	Determination of the binding affinity for drug receptor complexes at the full atomistic level using solute tempering and multiple Bennett acceptance ratio : the case of FKBP12 tacrolimus related ligands	144.000	IBMPower6,
B	Maria Clelia	RIGHI	Universita' di Modena e Reggio and Centro S3, CNR Istituto di Nanoscienze	Understanding the kinetics of tribochemical reactions	150.000	IBMPower6,
B	Roberto	RIGHINI	University of Florence	Molecular dynamics calculation of two dimensional spectra	80.000	IBMPower6,
B	Carlo Andrea	ROZZI	Istituto Nanoscienze - CNR	Excited state electron dynamics in plastic solar cells	150.000	IBMPower6,
B	Paolo	RUGGERONE	University of Cagliari	Computational Study of the Interactions between Antibiotics and Ribosome	100.000	IBMPower6,
B	Alice	RUINI	University of Modena and Reggio Emilia	Designing Optoelectronic properties of pOlymer cRystals	121.000	IBMPower6,
B	Giacomo	SAIELLI	Istituto per la Tecnologia delle Membrane del CNR, Unita di Padova	Coarse-grained MD simulations of Ionic Liquid Crystals	130.000	IBMPower6,
B	PUNEET	SAXENA	University of Modena & Reggio Emilia	Targeting Opportunistic HIV co-infections: Design, synthesis & Biological Evaluation of Folate-dependent proteins	150.000	IBMPower6,
B	Tullio	SCOPIGNO	Universita' Sapienza	Dynamics and Thermodynamics of compressed liquid metals studied by ab-initio molecular dynamcs	61.440	BlueGene/P
B	Maurizio	SIRONI	Universita' di Milano	In silico design of FtsZ targetted antibacteric peptidomimetics	130.000	IBMPower6,
B	Gloria	TABACCHI	Universita' degli Studi dell'Insubria	Organic-inorganic hybrid dye-zeolite materials	100.000	IBMPower6,
B	Adrian	TOMPKINS	The Abdus Salam International Centre for Theoretical Physics (ICTP)	ultra high resolution Climate projections for Health Including Malaria risk in EasteRn Africa	120.000	IBMPower6,
B	Daniele	VARSANO	Univerista di Roma "La Sapienza"	ENVironmental effects on ELectronic and OPTical properties of biological chromophores: the case of PCP	150.000	IBMPower6,
B	Franco	VAZZA	Jacobs University Bremen, Radio Astronomy Institute - Bologna	Cosmic Rays in Simulated Galaxy Cluster with Adaptive Mesh Refinement	150.000	IBMPower6,