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**QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials**

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1605	Organic-inorganic compounds with strong nonlinear optical properties based on 2,4,6-trimethylpyridinium and tetrahedral BF <sub>4</sub> <sup>-</sup> networks. <b>2011</b> , 83,		5
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1603	Investigation of thermoelectric properties of chalcogenide semiconductors from first principles. <b>2011</b> , 109, 123712		25
1602	First-principles calculations of <sup>17</sup> O nuclear magnetic resonance chemical shielding in Pb(Zr(1/2)Ti(1/2))O <sub>3</sub> and Pb(Mg(1/3)Nb(2/3))O <sub>3</sub> : linear dependence on transition-metal/oxygen bond lengths. <b>2011</b> , 135, 114507		5
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1598	Highly spin-polarized conducting state at the interface between nonmagnetic band insulators: LaAlO <sub>3</sub> /FeS <sub>2</sub> (001). <b>2011</b> , 107, 166601		27
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1586	Structural and thermodynamic properties of compressed palladium: Ab initio and molecular dynamics study. <b>2011</b> , 83,		33
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1574	Bond disorder and breakdown of ballistic heat transport in the spin-12 antiferromagnetic Heisenberg chain as seen in Ca-doped SrCuO <sub>2</sub> . <b>2011</b> , 84,	16
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1554	Electronic structure and stability of layered superlattice composed of graphene and boron nitride monolayer. <b>2011</b> , 83,	45
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1550	Phonon, two-magnon, and electronic Raman scattering of Fe <sub>1+y</sub> Te <sub>1-x</sub> S <sub>x</sub> . <b>2011</b> , 83,	40
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1536	Quantum size effects on chemisorption properties: CO on ultrathin Cu films from first principles. <b>2011</b> , 84,	3
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1534	Correlation energy functional from jellium surface analysis. <b>2011</b> , 84,	36
1533	Vibrational spectrum and electron-phonon coupling of doped solid picene from first principles. <b>2011</b> , 84,	53
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1526	Thermoelectric transport properties of silicon: Toward an ab initio approach. <b>2011</b> , 83,		49
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1431	X-ray absorption spectra of In <sub>x</sub> Ga <sub>1-x</sub> N alloys with insight from atom-specific simulations. <b>2012</b> , 86,	3
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1428	Ab initio investigation of defect formation at ZrO <sub>2</sub> -CeO <sub>2</sub> interfaces. <b>2012</b> , 86,	15
1427	Formation of NaCl-type monodeuteride LaD by the disproportionation reaction of LaD <sub>2</sub> . <b>2012</b> , 108, 205501	15
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1419	Vibrational properties of alkyl monolayers on Si(111) surfaces: Predictions from ab-initio calculations. <b>2012</b> , 100, 071605	4
1418	Direct detection of sub-GeV dark matter. <b>2012</b> , 85,	291
1417	Prediction of a metastable phase of silicon in the Ibam structure. <b>2012</b> , 85,	36
1416	Geometrical frustration in the spin liquid $\beta$ -Me <sub>3</sub> EtSb[Pd(dmit) <sub>2</sub> ] <sub>2</sub> and the valence-bond solid Me <sub>3</sub> EtP[Pd(dmit) <sub>2</sub> ] <sub>2</sub> . <b>2012</b> , 109, 097206	34
1415	Enhanced carrier mobilities in two-dimensional electron gases at III-III/I-V oxide heterostructure interfaces. <b>2012</b> , 85,	25
1414	Phonon engineering in nanostructures: Controlling interfacial thermal resistance in multilayer-graphene/dielectric heterojunctions. <b>2012</b> , 101, 113111	45
1413	Identification of the nitrogen split interstitial (N-N)(N) in GaN. <b>2012</b> , 109, 206402	33
1412	Anomalous work function anisotropy in ternary acetylides. <b>2012</b> , 86,	13
1411	Generalized-gradient-approximation noninteracting free-energy functionals for orbital-free density functional calculations. <b>2012</b> , 86,	54
1410	Diffusion of hydrogen in Pd assisted by inelastic ballistic hot electrons. <b>2012</b> , 108, 115902	18
1409	Ab initio study of energy loss and wake potential in the vicinity of a graphene monolayer. <b>2012</b> , 86,	27
1408	Modeling the role of the fluorine dopant in the magnetic phase diagram of LaFeAsO <sub>1-x</sub> F <sub>x</sub> superconductors. <b>2012</b> , 85,	1
1407	Ordered arrays of size-selected oxide nanoparticles. <b>2012</b> , 108, 195507	20
1406	Optical phonon anomaly in Bernal stacked bilayer graphene with ultrahigh carrier densities. <b>2012</b> , 86,	3
1405	Nonuniform scaling applied to surface energies of transition metals. <b>2012</b> , 108, 126402	50
1404	Plane-wave transport method for low-symmetry lattices and its application. <b>2012</b> , 86,	6
1403	Magn $\pi$ -like phases in epitaxial anatase TiO <sub>2</sub> thin films. <b>2012</b> , 86,	22

1402	Quantum Monte Carlo study of pressure-induced B3B1 phase transition in GaAs. <b>2012</b> , 86,	8
1401	Structure and intermolecular bonding in NaBH <sub>4</sub> ·2H <sub>2</sub> O: A density functional theory study. <b>2012</b> , 85,	2
1400	Optical properties of the iron-pnictide analog BaMn <sub>2</sub> As <sub>2</sub> . <b>2012</b> , 86,	12
1399	Unraveling the polar state in TMTTF <sub>2</sub> -PF <sub>6</sub> organic crystals. <b>2012</b> , 85,	11
1398	Unconventional magnetism as a consequence of the charge disproportionation and the molecular orbital formation in Ba <sub>4</sub> Ru <sub>3</sub> O <sub>10</sub> . <b>2012</b> , 86,	35
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1396	Electron-phonon coupling and superconductivity in arsenic under pressure. <b>2012</b> , 86,	14
1395	Carbon rehybridization at the graphene/SiC(0001) interface: Effect on stability and atomic-scale corrugation. <b>2012</b> , 85,	29
1394	Comment on Observation of anomalous peaks in the photoelectron spectra of highly oriented pyrolytic graphite: Folding of the band due to the surface charge density wave transition. <b>2012</b> , 85,	
1393	Strain-activated edge reconstruction of graphene nanoribbons. <b>2012</b> , 85,	23
1392	Pressure-driven evolution of the covalent network in CaB <sub>6</sub> . <b>2012</b> , 109, 075501	46
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1389	First-principles study of the atomic and electronic structures of misfit-layered calcium cobaltite (Ca <sub>2</sub> CoO <sub>3</sub> )(CoO <sub>2</sub> ) <sub>1.62</sub> using rational approximants. <b>2012</b> , 85,	37
1388	Thermalization of photoexcited carriers in bismuth investigated by time-resolved terahertz spectroscopy and ab initio calculations. <b>2012</b> , 85,	26
1387	Virtual-crystal approach to aluminum-avoidance materials: A first-principles density-functional calculation of micas. <b>2012</b> , 85,	3
1386	First-Principles Study of the Influence of (110) Strain on the Ferroelectric Trends of TiO <sub>2</sub> . <b>2012</b> , 429, 31-42	7
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1384	Irradiation-induced formation of nanocrystallites with C15 Laves phase structure in bcc iron. <b>2012</b> , 108, 025501		100
1383	Local and nonlocal electron-phonon couplings in K3 picene and the effect of metallic screening. <b>2012</b> , 86,		22
1382	Band-edge levels in semiconductors and insulators: Hybrid density functional theory versus many-body perturbation theory. <b>2012</b> , 86,		62
1381	Adsorbate induced restructuring of TiO <sub>2</sub> (011)-(2 $\bar{1}$ ) leads to one-dimensional nanocluster formation. <b>2012</b> , 108, 106105		25
1380	First-principles calculation of the electron-phonon interaction in semiconductor nanoclusters. <b>2012</b> , 85,		25
1379	Resilience of gas-phase anharmonicity in the vibrational response of adsorbed carbon monoxide and breakdown under electrical conditions. <b>2012</b> , 86,		5
1378	Oxygen vibrations and acoustic surface plasmon on Be(0001). <b>2012</b> , 86,		15
1377	Chemical ordering in Cr <sub>3</sub> Al and relation to semiconducting behavior. <b>2012</b> , 86,		4
1376	Frequencies and polarization vectors of phonons: Results from force constants which are fitted to experimental data or calculated ab initio. <b>2012</b> , 86,		3
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1374	Ab initio analytical infrared intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method. <b>2012</b> , 137, 204113		115
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1371	Local structural models of complex oxygen- and hydroxyl-rich GaP/InP(001) surfaces. <b>2012</b> , 136, 064705		25
1370	First-principles molecular dynamics study on simple cubic calcium: comparison with simple cubic phosphorus. <b>2012</b> , 32, 11-17		1
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1351	Coherent phonon heat conduction in superlattices. <b>2012</b> , 338, 936-9		403
1350	Oxidation of graphene in ozone under ultraviolet light. <b>2012</b> , 101, 073110		67
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1346	Ideal strength and phonon instability in single-layer MoS <sub>2</sub> . <b>2012</b> , 85,	274
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1329	Strain dependent polarization and dielectric properties of epitaxial BaTiO <sub>3</sub> from first-principles. <b>2012</b> , 112, 014109	10
1328	An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm. <b>2012</b> , 137, 224108	223
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1326	Phononic band gap engineering in graphene. <b>2012</b> , 112, 094307	12
1325	Electronic and vibrational signatures of Stone-Wales defects in graphene: First-principles analysis. <b>2012</b> , 86,	61
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1317	Structures and lattice energies of molecular crystals using density functional theory: Assessment of a local atomic potential approach. <b>2012</b> , 550, 94-98	19
1316	First-principles calculation of the bulk photovoltaic effect in bismuth ferrite. <b>2012</b> , 109, 236601	166
1315	Optical properties of an organic dye from time-dependent density functional theory with explicit solvent: the case of alizarin. <b>2012</b> , 137, 154314	17
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1313	Optical properties of calcium under pressure from first-principles calculations. <b>2012</b> , 86,	5

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1295	First-principles study of electronic and dynamical properties of the TaC(001) surface. <b>2012</b> , 25, 19-23	4

1294	First principles study of dielectric and vibrational properties of pyrochlore hafnates. <b>2012</b> , 14, 1405-1411	26
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1268	Electron-phonon coupling in crystalline organic semiconductors: microscopic evidence for nonpolaronic charge carriers. <b>2012</b> , 109, 126407		29
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1260	High-pressure phases of lithium borohydride LiBH <sub>4</sub> : A first-principles study. <b>2012</b> , 86,		16
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1255	Dynamic ionic clusters with flowing electron bubbles from warm to hot dense iron along the Hugoniot curve. <b>2012</b> , 109, 175701		28
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