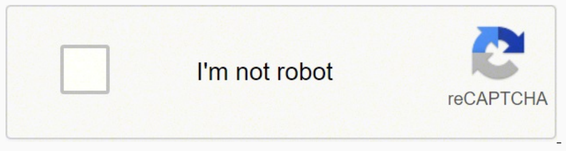

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Release notes elk-8.4.6 -fixed problem with real-time TDDFT restarts (tasks 461 and 463); this problem occurred only very rarely for systems with particular symmetries; thanks to Antonio Sanna for finding this -added batch calculations as a new feature; with this Elk can perform multiple runs while adjusting a particular parameter -- for example producing an energy vs volume plot; see the examples in elk/examples/batch-calculations -input and output variables will be added to batch calculations upon request -Yunfan Liang and Xavier Gonze discovered a problem in the non-linear optical response formalism of our work in Phys. Rev. B 67, 165332 (2003); consequently, the non-linear optics code has been completely re-written and throughly tested; see the example in /elk/examples/non-linear-optics -the speed ultra long-range calculations has been greatly improved thanks to changes in the generation of the long-range density and magnetisation -several minor bug fixes, optimisations and improvements -Elk has been recognized with a Community Choice award by SourceForge; thanks to all the users and contributors for making the code as useful as it is, as well as for making the forums a congenial place for everyone elk-8.3.22 -fixed a bug which occurred when using the OpenBLAS library with Elk's RAM disk feature; thanks to Marcin Dulak for finding this elk-8.3.20 -included missing BLAS and LAPACK files in the package; thanks to Jagdish Kumar for pointing out the omissions elk-8.3.15 -considerable speed-up and optimisations throughout the entire code; spin-polarised calculations in particular are substantially faster -greatly improved the meta-GGA calculations; these no longer require a large number of empty states for good convergence and consequently run much faster; removed the 'metagga' flag; thanks to Pietro Bonfa for the careful testing -checked and highly optimised the TDDFT+U calculations -removed the DFT+U scheme which interpolated between FLL and AFM -rearranged the order of phonon line width plots to match that of the phonon dispersion plots -further improved the electron-phonon Bogoliubov method; thanks to Chung-Yu Wang for the careful testing -rewrote much of the tensor moment code; the tensor moments are now real and exclusively of the 3-index type; the corresponding matrices Gamma_t^kpr are now Hermitian and orthonormal; see the documentation of the routines 'tm2todm' and 'tm3todm' and references therein; thanks to Leon Kerber for the extensive testing -writing out the old convention of complex 3-index tensor moments can be enabled with 'tm3old=.true.' -Leon Kerber also found and fixed a problem with the fixed tensor moment (FTM) code -the input block 'tmomfix' has been removed; use 'tm3fix' instead -included a FTM example in elk/examples/FeGd-fixed-tensor-moment -the RAM disk is now enabled by default; if problems are encountered with this then set 'ramdisk=.false.' -included an example for calculating the dielectric function using time evolution; see elk/examples/TDDFT-time-evolution/Si-dielectric -added more LaTeX documentation to the code -many small improvements and minor bug fixes elk-7.2.42 -added new RAM disk feature which allows Elk to store direct-access files in memory and can dramatically speed up calculations; enable this by setting 'ramdisk' to .true. in elk.in -many optimisations throughout the code -fixed an issue with the scissors operator in optical response code (task=320, 330, 331) for materials which are nearly metallic; thanks to Peter Elliott for pointing this out -further improved the electron-phonon mean-field code -added variables 'scalex', 'scaley' and 'scalez' to the input file; these allow scaling of the unit cell in the Cartesian directions elk-7.1.14 -optimised the second-variational procedure by changing the muffin-tin dot products to single-precision arithmetic; this speeds up this step by at least a factor of two for large systems without losing overall precision or stability -removed 'mixpack', 'phmixpack' and 'mixpacku' routines; Kohn-Sham potentials and fields are now stored in a single array accessed by pointer arrays; this removes the need for packing before and unpacking after mixing -increased speed of direct access reads by removing unnecessary 'close' statements -added an example for the ultra long-range method; see the input file in elk/examples/ultra-long-range/Cr-SDW/ -changed the Wannier90 .win file to improve the wannierisation convergence rate -fixed several bugs in the electron-phonon mean-field method -updated BLAS and LAPACK to version 3.9.0 -minor improvements and bug fixes elk-7.0.12 -Chung-Yu Wang added electron-phonon mean-field theory; this is a new method and still highly experimental -Alyn James wrote an interface for Elk to the DMFT code TRIQS; this interface is maintained in a separate branch of the Elk code found here. -fixed serious problem with DFT+U for dftu=3 (interpolation of FLL and AFM); this bug was introduced some time ago; we recommend that you check any previous calculations which use dftu=3 -lots of optimisations throughout the code -further improved Ehrenfest dynamics -added the calculation of Born effective charges using Ehrenfest dynamics (task=478); this is intended as a test for the method; Born effective charges are more accurately calculated with the King-Smith and Vanderbilt method (task=208) -Pietro Bonfa found and fixed several problems with the calculation of Mössbauer hyperfine fields -PB also added a new Mössbauer example: antiferromagnetic NiF2; see the examples/Mossbauer/NiF2 directory -Ronald Cohen fixed a bug in iso-volumetric lattice optimisation -RC also discovered a problem with the Wu-Cohen '06 GGA functional which has now been fixed -RC also suggested an efficiency improvement to the non-linear optics code -added tests for non-linear optics -Antonio Sanna helped fix a bug with TD forces -Karel Carva discovered that lmaxo should be at least 7 for phonopy calculations -change the default ntswrite from 10 to 500 time steps in order to reduce I/O -confirmed compatibility with Libxc version 5.1.0 -Further improved the ultra long-range code; the method has now been published: elk-6.8.4 -Born effective charges using the method of R. D. King-Smith and David Vanderbilt, Phys. Rev. B 47, 1651(R) (1993) are now available; see the directory elk/examples/Born-effective-charge -added Ehrenfest dynamics to the code; see the directory elk/examples/TDDFT-time-evolution/FeCo-Ehrenfest (highly experimental) -upgraded code to be compatible with Libxc version 5; note changes to the make.inc file -the Libxc SCAN functional no longer works with Elk, the regularised version of A. P. Bartók and J. R. Yates, J. Chem. Phys. 150, 161101 (2019) works and should be used instead; see the meta-GGA examples -Aldo Romero and his group interfaced PyProcar to Elk and confirmed that it worked with non-collinear magnetism; PyProcar is a robust, open-source Python library used for pre- and post-processing of the electronic structure data from DFT calculations -implemented a great many optimisations throughout the entire code; more aggressive use of the stack instead of the heap, this may require the user to increase the stack space -added the incomplete basis set (IBS) correction to forces from time-dependent vector potential, A(t) -fixed bug related to lattice optimisation with non-symmorphic symmetries thanks to Andrew Shyichuk and Jack Whaley-Baldwin; see here -added several new tests, including one for the stress tensor -updated physical constants to CODATA 2018 -fixed wavefunction and STM plotting thanks to Andrew Shyichuk -fixed bug in GW band structure code thanks to Antik Sihi -fixed problem with fixed tensor moment calculations -fixed problem in TDDFT real-time restart thanks to Peter Elliott -Peter Elliott and JKD also added Maxwell's equations for the macroscopic induced vector potential -updated and improved the ultra long-range code -forces are now written during a TDDFT run every 'ntsforce' time steps -matrix sizes larger than those addressable with four byte integers can now be used with BSE and MPI -Hartree-Fock information is now written to HF_INFO.OUT rather than INFO.OUT -parallelised the Brillouin zone integration (brzint) which considerably speeds up DOS calculations -modified how the potential of the optimised effective potential (OEP) iteration scheme is initialised -removed obsolete command from ProTex Perl script -added tests for Libxc and MPI; run 'make test-libxc' and 'make test-MPI' respectively, or 'make test-all' to test everything -fixed problem with hybrid functionals introduced a few versions back; also added a test for hybrids elk-6.3.2 -very large speedup of the first-variational Hamiltonian and overlap matrix setup; this is particularly apparent for large systems -made all of the numerical radial integrals much more efficient by storing the spline integration weights; this speeds up most of the code -switched radial integral infinitesimal from 1/3 d(r^3) to r^2dr; this improves numerical accuracy and returns to the convention of version 5.2.14 -added full (l,m) and spin characters for plotting the band structure with so-called 'fat bands'; these are performed with new tasks 22 and 23; thanks to Jagdish Kumar for the suggestion -Jagdish Kumar also fixed a problem with the phonon thermodynamic quantities which had an unnecessary prefactor of the number of atoms; see here -fixed a problem with occurs with constant electric fields (when efieldc is made finite) and crystals with non-symmorphic symmetries -Michael Fechner improved the fixed spin moment code by removing the requirement that unspecified muffin-tin fixed moments are checked for symmetry compliance -added 1D plotting of the magnetisation density, exchange-correlation magnetic field, electric field and m(r) x B_xc(r) with tasks 71, 81, 141 and 151, respectively -added density, potential and magnetisation plotting for ultra long-range calculations with tasks 731, 732, 733, 741, 742, 743, 771, 772 and 773 -constant electric fields can now be included in ultra long-range calculations; this can be done by setting the vector efielduc -an arbitrary external Coulomb potential can now be read in for use in the ultra long-range calculations; set trdvclr=.true. and the potential is read from the file VCLR.OUT elk-6.2.8 -Wannier90 interface added thanks to Arsenii Gerasimov, Yaroslav Kvashnin and Lars Nordström; and based on the original work of Duc Le and Jon Lafuente Bartolomé -the Wannier90 interface can be used to produce Hartree-Fock band structures (see example) and also works with non-collinear spin-polarised calculations -ultra long-range (ULR) calculations now available thanks to Tristan Müller (experimental) -self-consistent density GW calculations now available thanks to Arkardy Davydov and others; this is a new method still undergoing testing and is thus experimental -GW density matrix can now be written to file with task=640; the natural orbitals and occupation numbers are written to EVECSV.OUT and OCCSV.OUT, respectively -classical spin and orbital dipole magnetic fields can now be calculated and added to the Kohn-Sham field (set tbdip=.true. and tcden=.true.) -extensive optimisations throughout the code: every task should be noticeably faster -improved OpenMP parallelism -improved accuracy of the Mössbauer hyperfine field calculations -added spin and orbital dipole terms to the hyperfine field -updated constants and conversion factors to CODATA 2018 -added Andrew Shyichuk's improved check for requirement of the Tran-Blaha constant -variational meta-GGA functionals (like SCAN) now work with forces -added Roger Mason's fix to make FFTW thread-safe -René Wirnata has created the Elk Optics Analyzer that helps to visualize and post-process optics output data -regenerated species files with lower order local-orbitals -improved k-point convergence of the electron-phonon coupling constant for calculation of superconducting properties -upgraded to LAPACK 3.8.0 -changed default 'radkpt' from 30 to 40 -many minor improvements and bug fixes elk-5.2.14 -Youzhao Lan found a bug which prevented potential-only meta-GGA functionals (like Tran-Blaha) from being used; this has now been fixed -fixed meta-GGA atomic forces; thanks to Michael Porer for pointing out the problem -Eike Schwier discovered a conflicting MPI variable name and also reported that the code crashes when generating species files; both problems are now fixed -linear-response TDDFT off-diagonal components for q=0 now available (experimental) elk-5.2.10 -GW code is much improved and also faster; the Pade analytic continuation of the self-energy is more stable and reliable -OpenMP parallelism greatly improved; nesting is now permanently switched on and the number of threads is controlled by Elk itself; this should improve scaling on hundreds of CPU cores; please report any problems you have with parallelism on the forum -GW spectral function band-structures are now possible, such as this for silicon: ...these calculations are very expensive; the above example took around 600 CPU days; but will work for insulators, metals, non-collinear magnetic systems and so on; this feature is still experimental -Yaroslav Kvashnin and Lars Nordström found and fixed a bug in the fixed spin moment direction code -fully variational meta-GGA (in the generalised Kohn-Sham sense) is now running in conjunction with Libxc (experimental) -variational meta-GGA works only with collinear magnetism; let us know if you have an idea on how to extend it to the non-collinear case -Elk now interfaces to Libxc version 4 -- please update your library from version 2 -gauge invariant current density plots in 2D and 3D now available (tasks 372 and 373) -the entire code is much faster, particularly advanced methods like Hartree-Fock, RDMFT, BSE and GW; this is in part due to a 'coarse' Fourier grid for the wavefunctions -the lmaxi has been changed from 3 to 1 and several optimisations based on this have been hard-coded into Elk -Broyden mixing (mixtype=3) is now the default; magnetic calculations will now converge using a small bfieldc or bfcmt thanks to an improved magnetisation initialisation scheme -real-time TDDFT calculations no longer require 'nosym=.true.' but rather 'tshift=.false.' and are much faster as a consequence -2D and 3D current density plotting now available with tasks 272 and 273, respectively -task 480 generates a linear-response dielectric function calculation from a time-evolution run -lots of optimisations everywhere in the code, including additional OpenMP directives -lots of minor improvements and bug fixes -cleaned up and improved examples -several direct access files are not closed after reading which speeds up file I/O; please report any problems with this on the forum

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