The Improvement on GRASP2018 and its Computational Application in Precision Atomic Spectroscopy

Kai Wang[a,b]

[a] kaiwangcn@foxmail.com, *Department of Physics and Anhui Key Laboratory of Optoelectric Materials Science and Technology,Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Normal University, Wuhu, Anhui 241000, China*

[b]*Hebei Key Lab of Optic-electronic Information and Materials, The College of Physics Science and Technology, Hebei University, Baoding 071002, China*

Employing two state-of-the-art methods, multiconfiguration Dirac-Hartree-Fock [1] and second-order many-body perturbation theory [2], level energies, wavelengths, electric dipole, magnetic dipole, electric quadrupole, and magnetic quadrupole transition rates, oscillator strengths, and line strengths are calculated for a number of L- and M-shell ions of iron group elements for astrophysics interest [3-11]. Extensive comparisons with experiments from the NIST [12] and CHIANTI [13] databases, and other recent benchmark calculations, show that the present results are highly accurate: for excitation energies, uncertainty is less than 0.1% for most states; for transition rates, uncertainty is better than 10% for a majority of transitions.

The excellent description of energy separations along the isoelectronic sequence makes it possible to point out a number of lines for which experimental identifications are questionable. A complete dataset should be helpful in analyzing new observations from the sun and other astrophysical sources, and is also likely to be useful for modeling and diagnosing astronomical and fusion plasmas.

References

[1] C. Froese Fischer, M. Godefroid, et al., J Phys B, 49, 182004 (2016).
[2] M. F. Gu, Astrophys J, 169, 154 (2007).
[3] K. Wang, P. Jönsson, et al., Astrophys J Suppl S, 246, 1 (2020).
[4] K. Wang, P. Jönsson, et al., Astrophys J Suppl S, 235, 27 (2018).
[5] K. Wang, P. Jönsson, et al., Astrophys J Suppl S, 239, 30 (2018).
[6] K. Wang, P. Jönsson, et al., Astrophys J Suppl S, 229, 37 (2017).
[7] R. Si, S. Li, et al., Astrophys J Suppl S, 227, 16 (2016).
[8] K. Wang, Z. B. Chen, et al., Astrophys J Suppl S, 226, 14 (2016).
[9] K. Wang, R. Si, et al., Astrophys J Suppl S, 223, 3 (2016).
[10] K. Wang, X. L. Guo, et al., Astrophys J Suppl S, 218, 16 (2015).
[11] K. Wang, D. F. Li, et al., Astrophys J Suppl S, 215, 26 (2014).
[12] A. Kramida, Yu. Ralchenko, J. Reader, & NIST ASD Team, NIST. Atomic Spectra Database (ver. 5.3), [Online]. Available: http://physics.nist.gov/asd.
[13] P. R. Yong, K. P. Dere, et al., J Phys B, 49, 74009 (2016).