Abstract Submitted
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Low-Energy Electron Collisions with Copper and Gold Atoms[1]
KLAUS BARTSCHAT, OLEG ZATSARINNY, Drake University — We have extended the B-spline R-matrix (close-coupling) method [1] to fully account for relativistic effects in a Dirac-Coulomb formulation [2]. The computer code was applied to electron-impact excitation of the $(3d^{10}4s)^2S_{1/2} \rightarrow (3d^{10}4p)^2P_{1/2,3/2}$ and $(3d^{10}4s)^2S_{1/2} \rightarrow (3d^9 4s^2)^2D_{5/2,3/2}$ transitions in Cu and the corresponding transitions $(5d^{10}6s)^2S_{1/2} \rightarrow (5d^{10}6p)^2P_{1/2,3/2}$ and $(5d^{10}6s)^2S_{1/2} \rightarrow (5d^9 6s^2)^2D_{5/2,3/2}$ in Au. Our numerical implementation of the close-coupling method enables us to construct term-dependent, non-orthogonal sets of one-electron orbitals for the bound and continuum electrons. This is a critical aspect in the present problems, especially for the outermost d and s orbitals. Furthermore, core-polarization effects are accounted for *ab initio* rather than through a model potential. Our results will be compared with recent experimental data [3] and predictions from other theoretical approaches [4]. [1] O. Zatsarinny, Comp. Phys. Commun. **174**, 273 (2006). [2] O. Zatsarinny and K. Bartschat, Phys. Rev. A **77**, 062701 (2008). [3] M. Maslov, P.J.O. Teubner, and M.J. Brunger, Phys. Rev. A **77**, in press (2008). [4] D.V. Fursa, I. Bray, and R.P. McEachran, private communication (2008).

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