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First Principles Absorption Spectra of Cu_n ($n = 1 - 10$) Clusters KOPINJOL BAISHYA, JUAN C. IDROBO, SERDAR OGUT[1], University of Illinois at Chicago, MINGLI YANG, KOBLAR A. JACKSON[2], Central Michigan University, JULIUS JELLINEK[3], Argonne National Laboratory — First principles optical absorption spectra, obtained within time-dependent density functional theory, for the ground state and low-energy isomers of Cu_n ($n = 1 - 10$) are presented. Overall our theoretical results exhibit good agreement with available experimental data. We analyze the orbital character of the optical excitations as a function of size and energy. Compared to noble metal clusters of Ag and Au in the same size range,[4] we find that Cu clusters have much higher d-electron contribution to low-energy optical excitations.

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[4]J. C. Idrobo *et al.* Phys. Rev. B **76**, 205422 (2007); K. Baishya *et al. ibid.* **78**, 075439 (2008).

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