Title

Assessing the electronic properties of bimetallic complexes with N-M-N-M cycle (M = Ag, Au and Cu)

Abstract

This work is a theoretical study of the electronic properties of the reported bimetallic complexes M2(Ms(CH2SCN)3)2 (where M = Cu+, Ag+, Au+) coordinate with Ms(CH2SCN)3 ligand acting simultaneously as a bidentate chelate and bridge. The electronic properties were studied using reactivity indexes, Fukui function, NICS indexes showing that the metal is susceptible to a nucleophilic attack, whereas the nitrogen and sulfur ligand are susceptible to an electrophilic attack, and that the Phenyl ring aromaticity does not change with the metallic size. The absorption properties were studied via TD-DFT methods incorporating the relativistic scalar and spin–orbit correction. The most intense transitions are mainly localized in the visible region of the spectrum with a Metal to Ligand Charge Transfer (MLCT) character. The metal/ligand interactions were studied via the Morokuma-Ziegler decomposition scheme and Natural Orbital of Chemical Valence (NOCV). The three complexes might act as photocatalyst due to their visible light absorption observed transitions.

Authors

Zarate X.; Treto-Suárez M.A.; Hidalgo-Rosa Y.; Schott E.

Author full names

Zarate, Ximena (25653306000); Treto-Suárez, Manuel A. (57194466702);

Hidalgo-Rosa, Yoan (57210552565); Schott, Eduardo (12766226900)

Author(s) ID

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Affiliations

Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Santiago, Chile; Departamento de Física y Química, Facultad de Ingeniería, IDETECO, Universidad Autónoma de Chile, Av. Alemania 01090, Temuco, 4810101, Chile; Centro de Nanotecnología Aplicada, Facultad de Ciencias, Ingeniería y Tecnología, Universidad Mayor, Camino La Pirámide 5750, Santiago, Huechuraba, Chile; Departamento de Química Inorgánica, Facultad de Química y de Farmacia, Centro de Energía UC, Centro de Investigación en Nanotecnología y Materiales Avanzados CIEN-UC, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna, Santiago, 4860, Chile

Authors with affiliations

Zarate X., Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Santiago, Chile; Treto-Suárez M.A., Departamento de Física y Química, Facultad de Ingeniería, IDETECO, Universidad Autónoma de Chile, Av. Alemania 01090, Temuco, 4810101, Chile; Hidalgo-Rosa Y., Centro de Nanotecnología Aplicada, Facultad de Ciencias, Ingeniería y Tecnología, Universidad Mayor, Camino La Pirámide 5750, Santiago, Huechuraba, Chile; Schott E., Departamento de Química Inorgánica, Facultad de Química y de Farmacia, Centro de Energía UC, Centro de Investigación en Nanotecnología y Materiales Avanzados

CIEN-UC, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna, Santiago, 4860, Chile

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Correspondence Address

X. Zarate; Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Santiago, Chile; email: ximena.zarate@uautonoma.cl

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