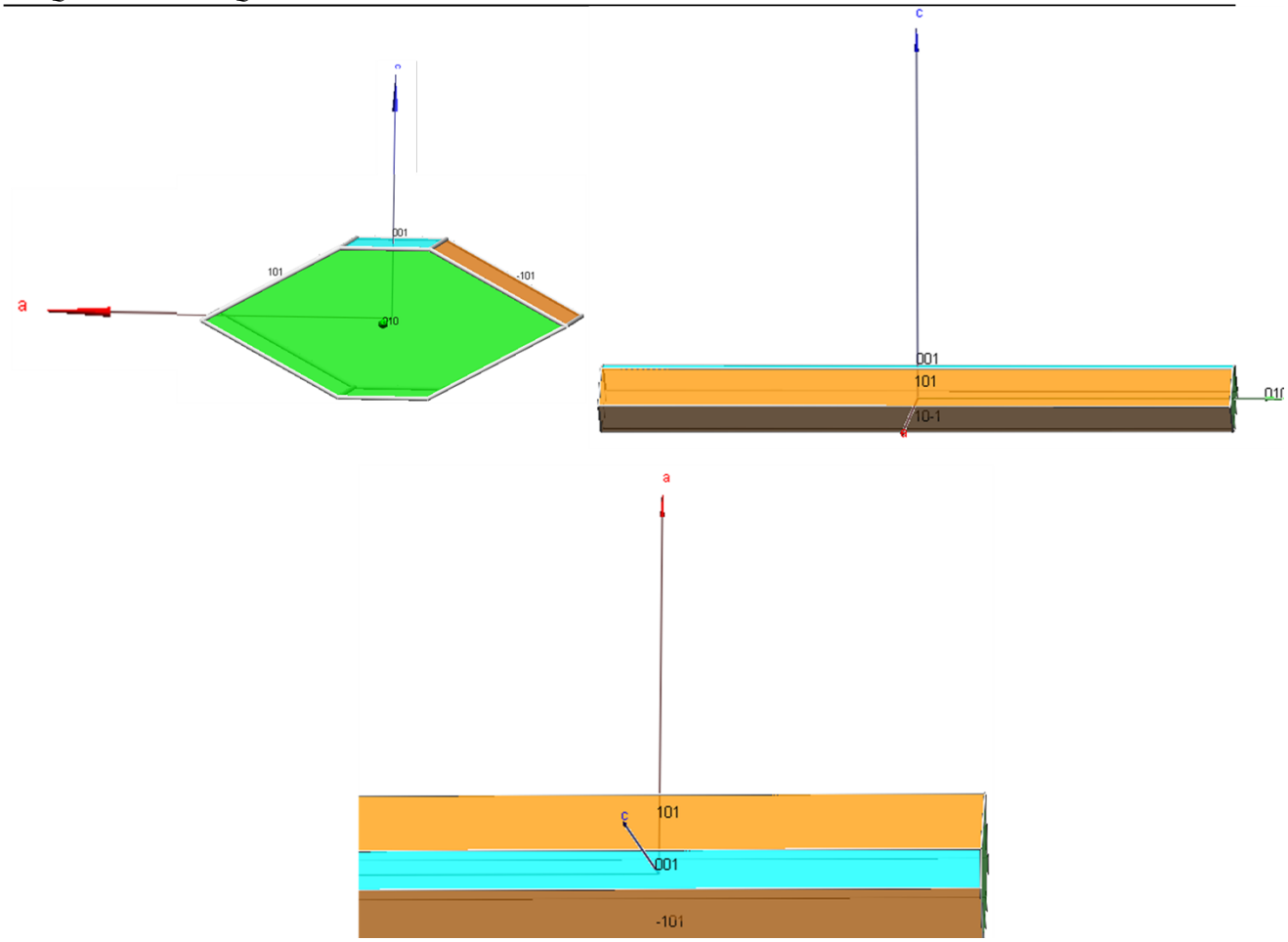
Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Support Information

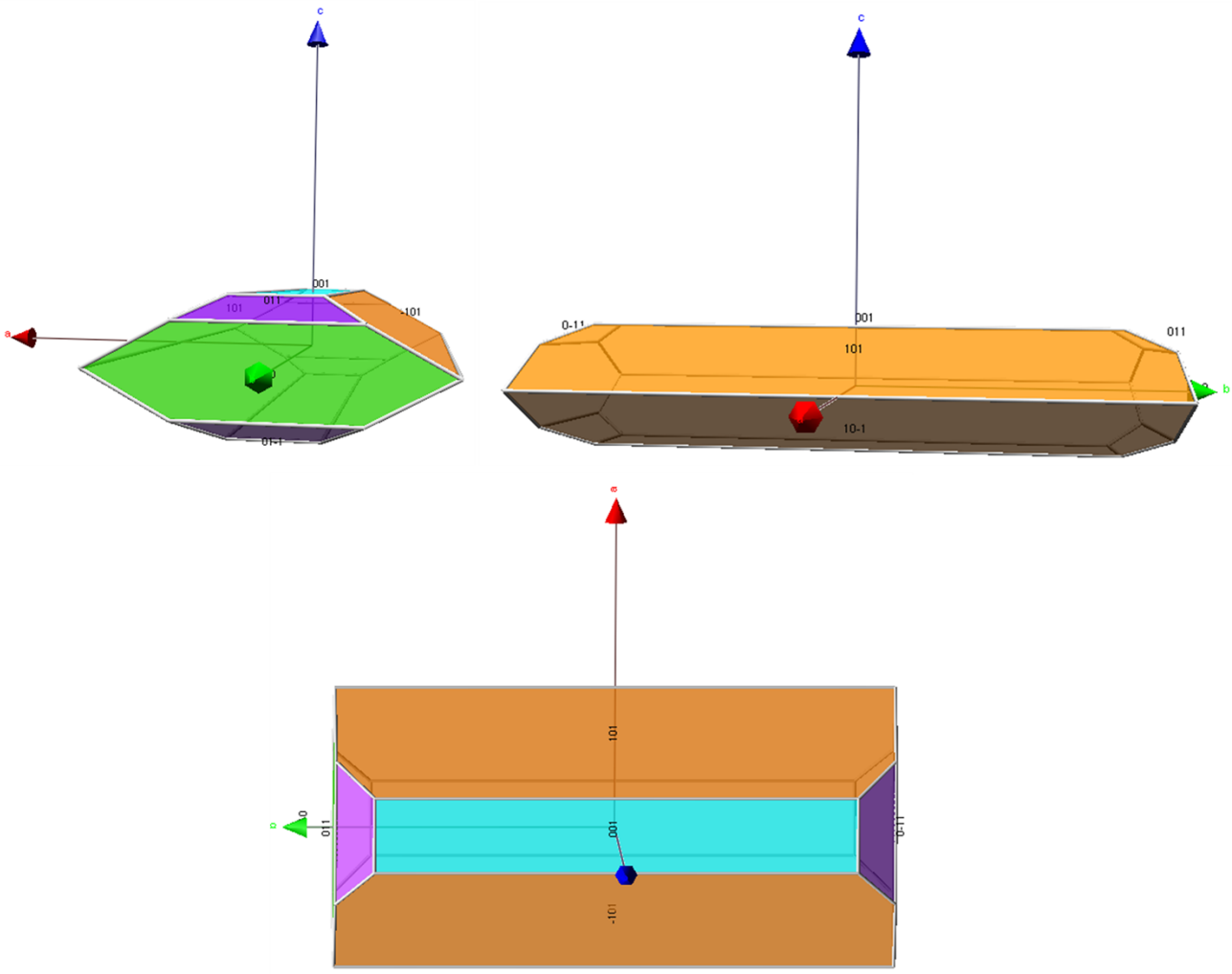
Facet-dependent photocatalytic and antibacterial properties in α–Ag_2WO_4 crystals: Combining experimental data and theoretical insights

R.A. Roca[a], J.C. Sczancoski[b], I.C. Nogueira[c], M.T. Fabbro[a,c], H.C. Alves[d], L. Gracia[e], L.P.S. Santos[c], C.P. de Sousa[d], G.E. Luz Jr.[f], J. Andrés[e], E. Longo[b], L.S. Cavalcante[f*]

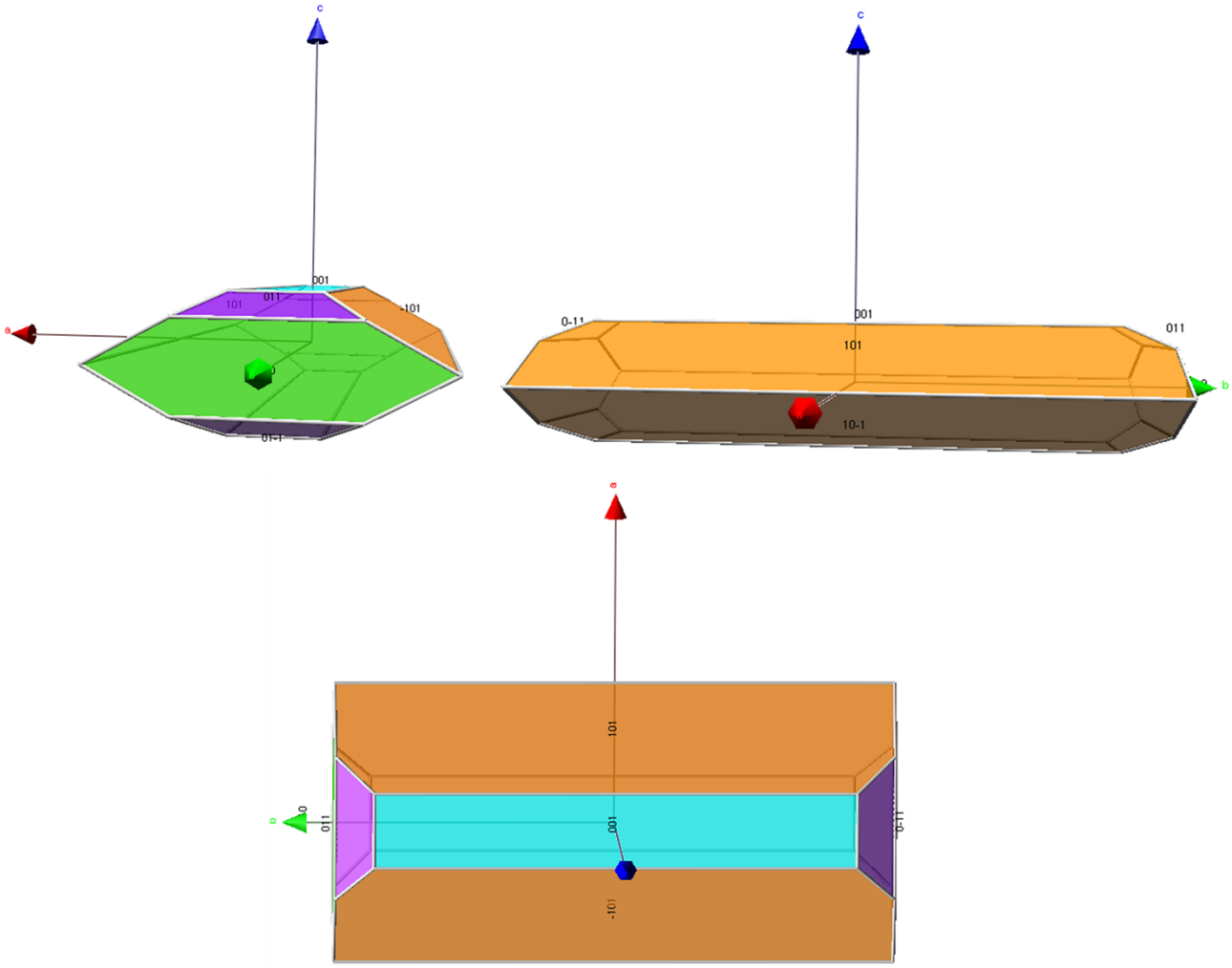
[a]*DQ-Universidade Federal de São Carlos, P.O. Box 676, 13565-905 São Carlos, São Paulo, Brazil*
[b]*CDMF-Universidade Estadual Paulista, P.O. Box 355, 14801-907, Araraquara, SP, Brazil*
[c]*Instituto Federal do Maranhão, Química e PPG em Engenharia de Materiais, 65025-001, 65030-005, São Luís, MA, Brazil*
[d]*Programa de Pós-Graduação em Biotecnologia, P.O. Box: 676, 13565-905, São Carlos, SP, Brazil*
[e]*Departamento de Química Física y Analítica, Universitat Jaume I (UJI), Castelló 12071, Spain*
[f]*PPGQ-GERATEC-CCN-DQ,Universidade Estadual do Piauí, João Cabral, N. 2231, P.O. Box 381, 64002-150 Teresina, PI, Brazil*



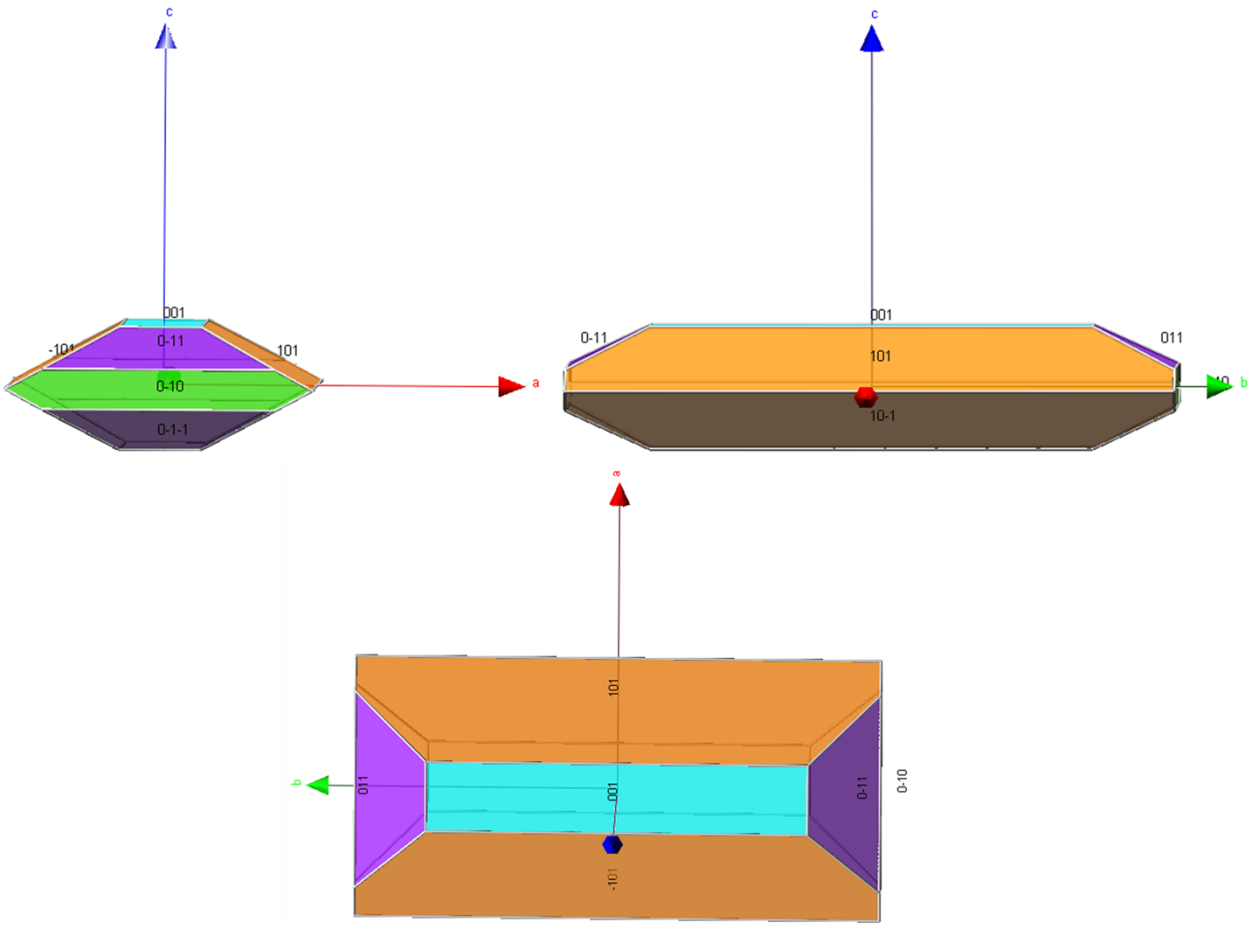
(a)



(b)



(c)



(d)

Fig. 1S(a–d). α–Ag_2WO_4 microcrystals at different perspectives of their crystallographic planes modeled from experimental data computationally.

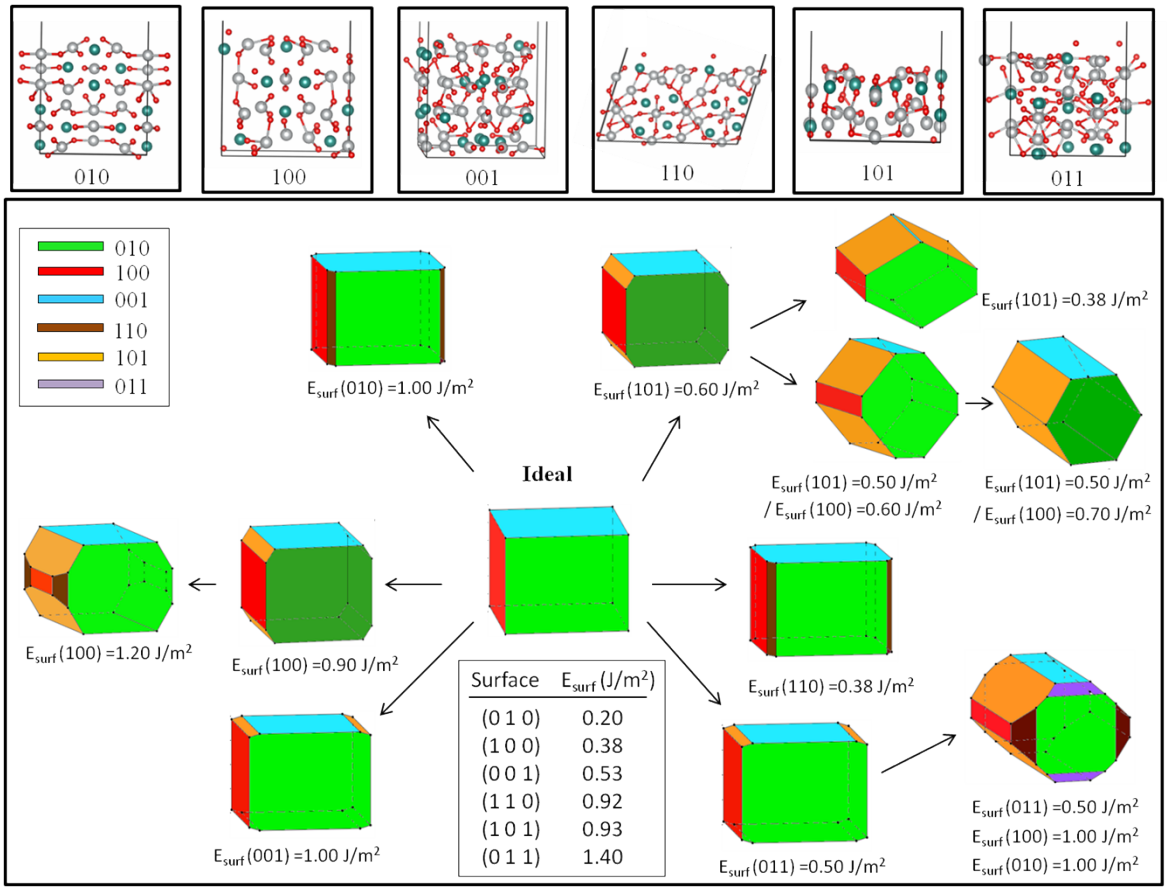


Fig. 2S(a). Crystals shape theoretical modeled by the Wulff theorem and their energy surface, respectively.

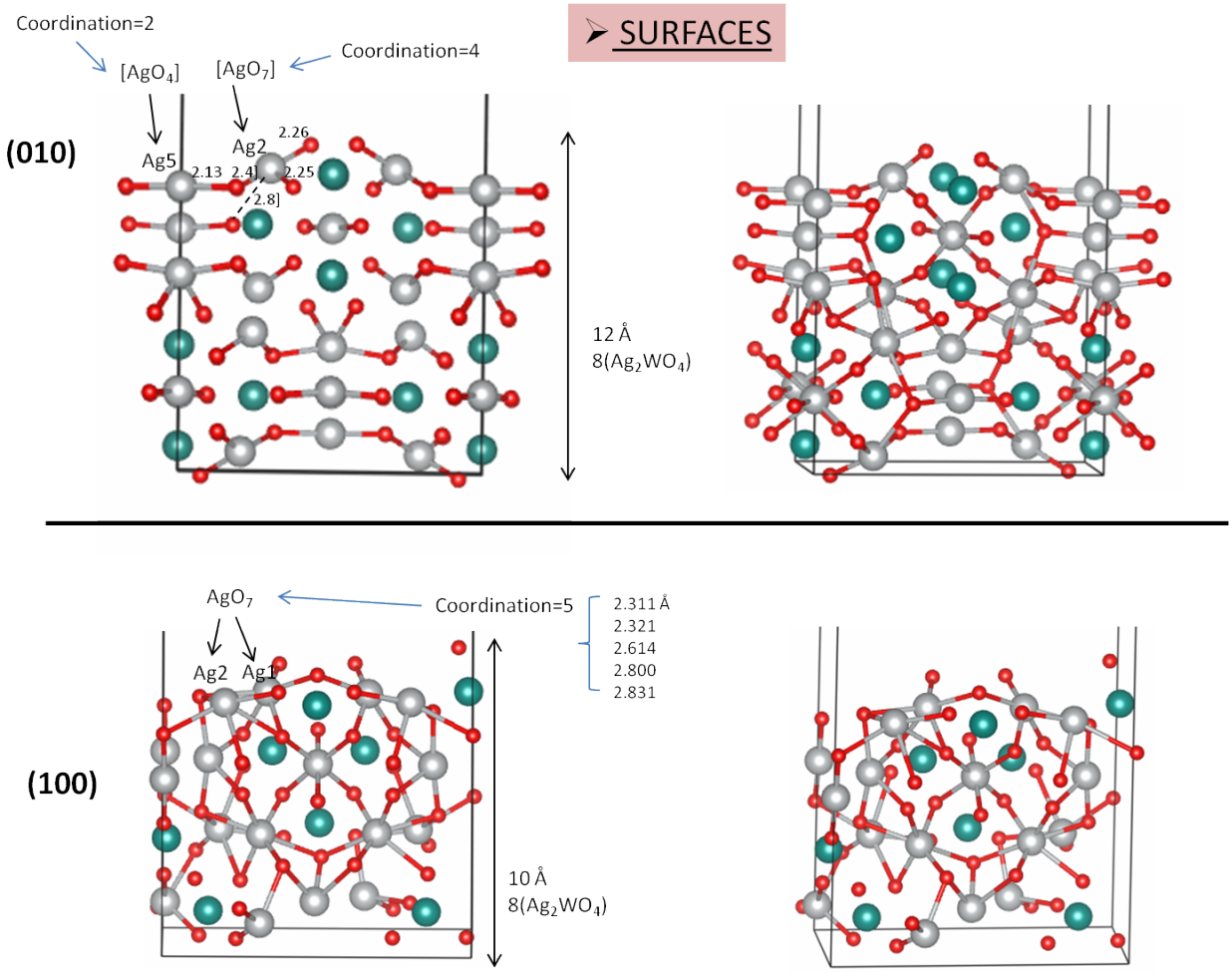


Fig. 2S(b). Clusters coordination and uncoordination numbers at (010) and (100) surfaces.

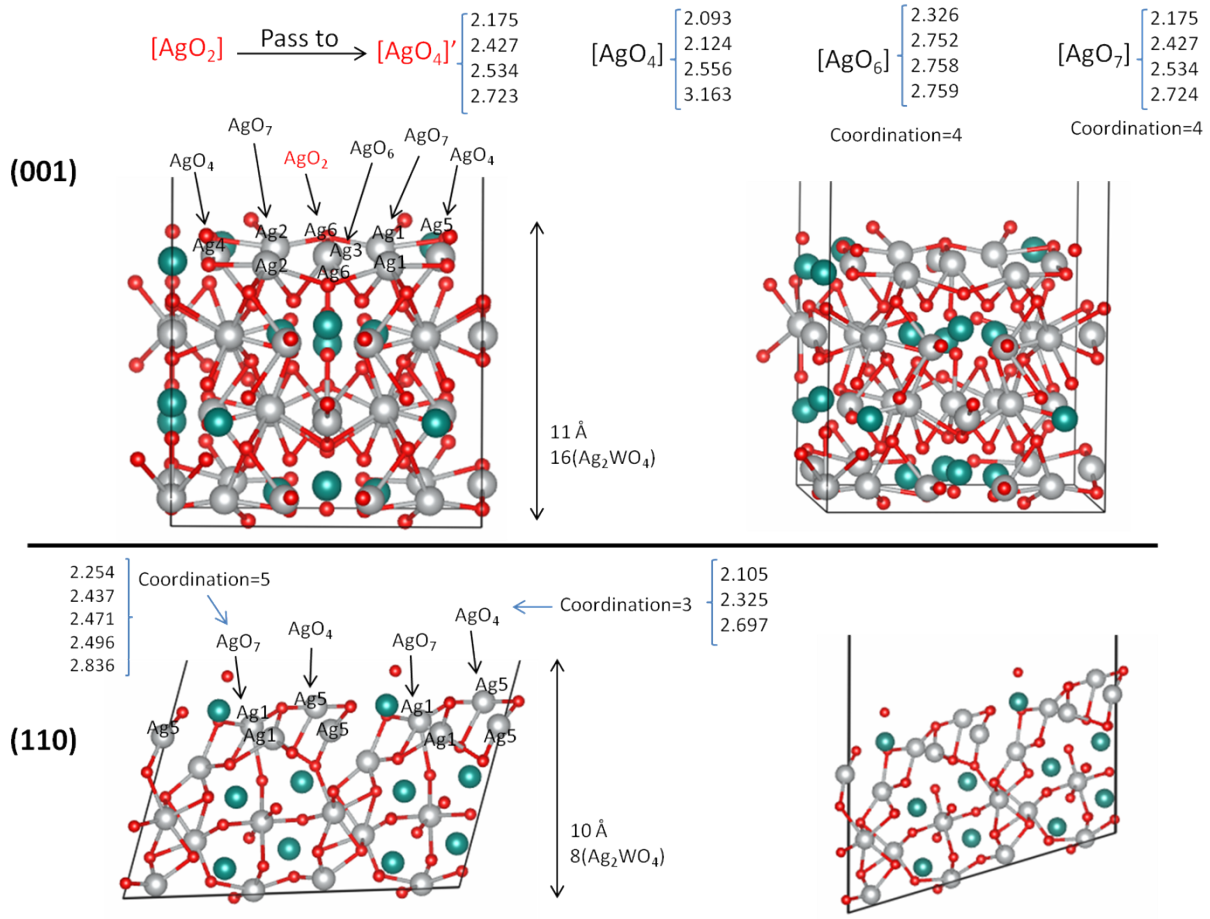


Fig. 2S(c). Clusters coordination and uncoordination numbers at (001) and (110) surfaces.

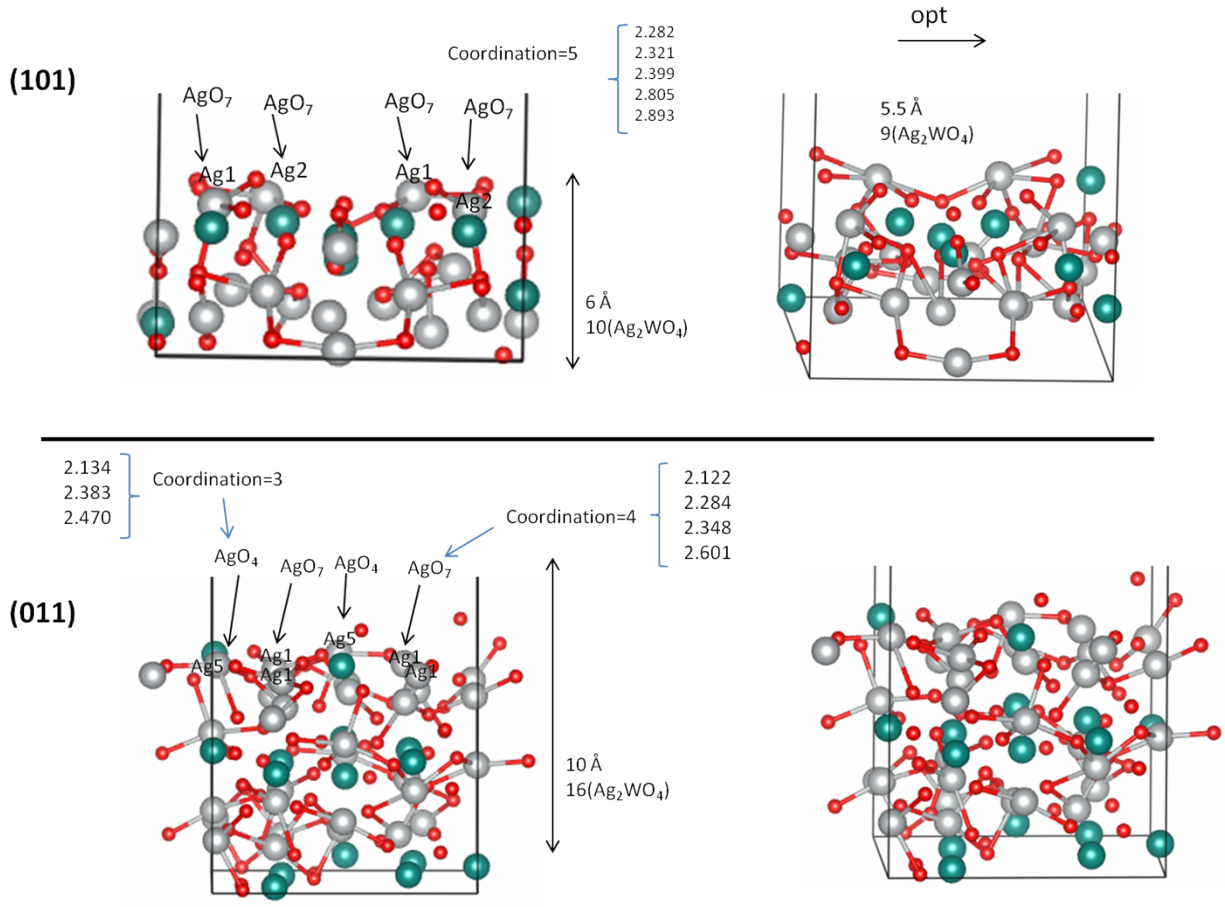


Fig. 2S(c). Clusters coordination and uncoordination numbers at (101) and (011) surfaces.