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On the possible role of organic matter in the transport/concentration of gold in geochemical environments; an atomistic and molecular approach

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The association of organic matter with ore minerals has been observed for many years. Over decades, many speculations have been proposed to define the possible roles that organic matter might have played in the ore genesis. In this paper [1], we performed a series of electronic calculations, and molecular dynamics simulations to investigate the behavior of organic matter in gold-forming environments.

Ab initio calculations revealed that Au-organic ligands are V-shaped complexes with an ionic head and a pair of non-ionic tails (see Figure, modified from [1]). The molecular dynamics and metadynamics simulations suggest that the organic Au-ligands are stable in both organic and aqueous phases, but are mostly posed at the interface of the organic-inorganic phase, in a way that its ionic head is placed in the aqueous solution, and its non-ionic tails are dissolved in the organic matter. Overall, this study suggests that the organic gold ligands thermodynamically prefer to pose at the nanoscale layer of interface between the organic and aqueous phases, which increases the concentration of gold at a very small portion of space and increases the possibility of the formation of a gold deposit.

[1] Haghi, A., Raissi, H., Hashemzadeh, H., & Farzad, F. (2022). On the role of alkanethiol Au complex in the formation of gold deposits; an in-silico approach. *Chemical Geology*, *610*, 121101.