

# Speciation and solubility of gold in CO<sub>2</sub>-HCl-H<sub>2</sub>O fluids: MD simulations and solubility experiments

WEIHUA LIU<sup>1</sup>, YUAN MEI<sup>1,2</sup>, JOËL BRUGGER<sup>2</sup>,  
ARTASHE MIGDISOV<sup>3</sup> AND ANTHONY WILLIAMS-JONES<sup>3</sup>

<sup>1</sup>CSIRO Mineral Resources Flagship, Melbourne,  
weihua.liu@csiro.au

<sup>2</sup>Monash University, Melbourne, Australia

<sup>3</sup>McGill University, Montreal, Canada

Increasing evidence of the abundance of water-poor, CO<sub>2</sub>-rich fluids in orogenic gold deposits indicates that 'exotic' volatile-rich fluids may have played a role in their formation (e.g., Ashanti Belt, Ghana [1]; Red Lake, Canada [2]; Sunrise Dam, Australia [3]). In water-rich, CO<sub>2</sub>-bearing fluids, CO<sub>2</sub> has been suggested to be a pH buffering agent, optimising gold solubility as gold-hydrosulphide complexes [4]. However, the role of CO<sub>2</sub> for gold mobility in water-poor, CO<sub>2</sub>-rich supercritical fluids is yet to be explored.

We have conducted preliminary gold solubility experiments and *ab initio* molecular dynamics simulations to investigate this problem. The solubility experiments have been conducted in a titanium autoclave at 340 °C with 0.01 m HCl, and the amount of water and CO<sub>2</sub> were loaded to the cell to ensure the fluid density is in the vapour phase with CO<sub>2</sub> mole fraction (CO<sub>2</sub>/(H<sub>2</sub>O+CO<sub>2</sub>)) ranging from 0.1 to 0.84. The results showed that gold solubility has a negative correlation to the CO<sub>2</sub> content in the fluids, i.e., decreasing with decreasing water fugacity.

*Ab initio* MD simulations of the AuCl<sup>0</sup> complex (linear [H<sub>2</sub>O-Au-Cl]<sup>0</sup>) in the CO<sub>2</sub>-H<sub>2</sub>O system were conducted at 340 °C with CO<sub>2</sub> mole fraction from 0.1-0.98 at densities between 0.78-0.15 g/cm<sup>3</sup>. The MD simulations indicate that the number of hydration water and H-bonds near the AuCl<sup>0</sup> complex decreases systematically with increasing CO<sub>2</sub> mole fraction. These results are consistent with the experiments, suggesting that H<sub>2</sub>O as a polarized molecule plays a more active role than the un-polarized CO<sub>2</sub> molecule in the fluids, and hydrated chloride species are the main form for transporting gold in the CO<sub>2</sub>-H<sub>2</sub>O-HCl system.

[1] Schmdit Mum et al., 1997, *Min. Dep.* **32**:107-118 [2] Chi et al., 2006, *Min. Dep.* **40**:726-741 [3] Baker et al., 2010, *Econ. Geol.* **105**:873-894 [4] Philips and Evans, 2004, *Nature*, **429**:860-863