

## Bonding properties of liquid Fe-Light-Element-O systems under high pressure: ab initio molecular-dynamics simulations

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Light elements (LE) such as hydrogen, carbon, oxygen, silicon, and sulfur are expected to exist in the Earth's core. For the liquid Fe-LE ternary systems which include two kinds of LE, several experimental and theoretical studies on the immiscibility of liquid Fe-Si-O [1-2] and Fe-S-O [3-4] ternary mixtures under high pressure have been reported. However, it is unclear the bonding properties of liquid Fe-LE-oxide ternary systems, which are the origins of various properties of liquids. For this reason, we have investigated the bonding properties of liquid iron-light-element-oxygen ternary systems such as Fe-H-O, Fe-C-O, Fe-Si-O, and Fe-S-O under high pressure by ab initio molecular dynamics simulations. Regarding the interactions between light elements, bond-overlap populations show covalent characters in C-C, Si-Si, and Si-O interactions in liquid Fe-C-O and Fe-Si-O even under high-pressure condition.

[1] Arveson, S.M., Deng, J., Karki, B.B., and Lee, K.K.M. (2019). *Proceedings of the National Academy of Sciences* 116, 10238.

[2] Huang, D., Badro, J., Brodholt, J., and Li, Y. (2019). *Geophysical Research Letters* 46, 6397-6405.

[3] Tsuno, K., Ohtani, E., and Terasaki, H. (2007). *Physics of the Earth and Planetary Interiors* 160, 75-85.

[4] Helffrich, G., and Kaneshima, S. (2004). *Science* 306, 2239-2242.

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