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Addition/Correction

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Correction to "Structural Evolution of Supercritical CO_2 across the Frenkel Line"

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In our recently published article,[1] text in the first paragraph starting on page 2786 should have explicitly indicated that it was quoted from a 2012 *Physics Today* article by Brazhkin and Trachenko.[2] In addition, a 2013 *Journal of Chemical Physics* paper by Bolmatov et al. (ref 3 here, ref 26 in the original publication) should have been cited at this point. Below is the corrected paragraph as it should have been originally published.

As pointed out by Brazhkin and Trachenko,[2] "gas particles move in almost straight lines until they collide with other particles or container walls and change course. In liquids, atomic motion has two components: a solid-like, quasiharmonic vibrational motion about equilibrium locations and diffusive jumps between neighboring equilibrium positions. As the temperature increases or the pressure decreases, a particle spends less time vibrating and more time diffusing. Eventually, the solid-like oscillating component of motion disappears; all that remains is the ballistic−collisional motion. That disappearance, a qualitative change in particle dynamics, corresponds to the transition of the substance from the liquid to the gas."[2,3] This smooth crossover at the Frenkel line is associated with the disappearance of the medium-range order correlations at high temperatures.[3] The disappearance of the second peak in the $g(r)$ profile ($g_{CC}(r)$, $g_{CO}(r)$) in the CO_2 simulations, shown in Figure 2c,d, corresponds to such a Frenkel line crossover change in local structure. The same was seen in the one-component Lennard-Jones (LJ) supercritical fluid.[3] The distribution function $g_{OO}(r)$ (see Figure 2a,b) exhibits unconventional behavior where medium-range order correlations remain robust and prevail over the short-range order over a very wide temperature range. This effect we attribute to localization of transverse-like phonon modes, which we will discuss in detail below.

We apologize for any inconvenience these errors may have cause our readers.

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REFERENCES

(1) Bolmatov, D.; Zav'yalov, D.; Gao, M.; Zhernenkov, M. Structural Evolution of Supercritical CO_2 across the Frenkel Line. *J. Phys. Chem. Lett.* **2014**, *5*, 2785−2790.

(2) Brazhkin, V. V.; Trachenko, K. What Separates a Liquid from a Gas? *Phys. Today* **2012**, *65*, 68−69.

(3) Bolmatov, D.; Brazhkin, V. V.; Fomin, Y. D.; Ryzhov, V. N.; Trachenko, K. Evidence for Structural Crossover in the Supercritical State. *J. Chem. Phys.* **2013**, *139*, 234501.

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