Supporting information

Novel silica filled deep eutectic solvent based nanofluids for energy transportation

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The supporting information document consists of 8 pages, 3 equations, and 3 figures.

Contents

1. Molecular dynamic Simulations method

Model and method

The molecular dynamics simulations were performed at 298 K under *NVT* (constant mass, volume and temperature) ensemble using LAMPPS. Working temperature was regulated by Nose-Hoover mothed [1]. The simulation time is 3 ns with a time step of 1 fs, resulting in the 3,000,000 simulation steps at each temperature and the last 1 ns of data was used for statistical analysis. The initial velocities of atoms were sampled according to Maxwell distribution. The velocities and positions of atoms along with the simulations were solved using Verlet velocity algorithm [2]. The Ewald method [3] and Atom-based [4] method were selected to calculate electrostatic interaction and Van der Waals interaction, respectively, with a cutoff distance of 12 Å. The ab-initio force field COMPASS (Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies) [5] was performed, of which rigorous force field parameters were obtained by using high level first principles.

Diffusion coefficient

The mean square displacement (MSD) is the statistical average of atoms trajectories with simulation time, which is used to characterize the diffusive behavior of system particles. The specific formula[6] is:

$$MSD = \left\langle \left| \vec{r}_i(t) - \vec{r}_i(0) \right|^2 \right\rangle \tag{S1}$$

where $\vec{r}_i(0)$ is the position vector corresponding to initial time and $\vec{r}_i(t)$ is the position vector at time *t*, and the angular brackets $\langle\ \rangle$ denote the ensemble average. Self-diffusion coefficient is one of important thermophysical properties that can characterize mass transfer phenomena and then guide the microscopic design for materials [7-9]. According to Einstein equation The self-diffusion

coefficient is expressed as follows [10]:

$$D = \frac{1}{6}\lim_{t\to\infty}\frac{d}{dt}\left\langle \left|\vec{r_i}(t) - \vec{r_i}(0)\right|^2 \right\rangle \quad \text{(S2)}$$

From the equation (S1) and (S2), the diffusion coefficient by this way equals the one-sixth of the slope of the MSD curves.

Radial distribution function

The radial distribution function (RDF) is the basic function characterizing liquid and disordered system. It describes the probability with a particle as the centre to find another particle within the spatial range from r to $r + dr$. RDF can depict distribution with distance of other particles around a particle. The radial distribution function can be defined:

$$x_\alpha x_\beta \rho g_{\alpha\beta}(\mathbf{r}) = \frac{1}{N}\left\langle \sum_{i=1}^{N_\alpha}\sum_{i=1}^{N_\beta}\delta\left(\mathbf{r} - \mathbf{r}_i + \mathbf{r}_j\right)\right\rangle \quad \text{(S3)}$$

where x_i is the mole fraction of atom group i, N_i is the number of atoms of atom group i, N denotes the total number of atoms, and ρ signifies the overall number density.

Hydrogen bond lifetime

the HB were counted based on the geometry rule [11] between HB donor and acceptor of the first frame trajectory. The lifetime of the hydrogen bonds means how long a hydrogen bond can exist. And the average hydrogen bonds lifetime of the entire system can be obtained by calculating the average of time from generation to disappearance of all hydrogen bonds.

Fig. S1 Stability study of chemically decorated silica filled DES based nanofluids. (a) Zeta potential of nanofluids with different types of nanoparticles (1.0 wt%); (b) Zeta potential of the nanofluids at different standing time; digital image of (c) SiO_2-SH-DP-Cu filled GL/ChCl DES based nanofluids (1.0 wt%), (d) SiO_2-SH-DP-Cu filled GL/ChCl DES based nanofluids (1.0 wt%) after putting at ambient temperature for 15 days; TEM image of nanofluids after standing for (e) 5 days and (f) 15 days.

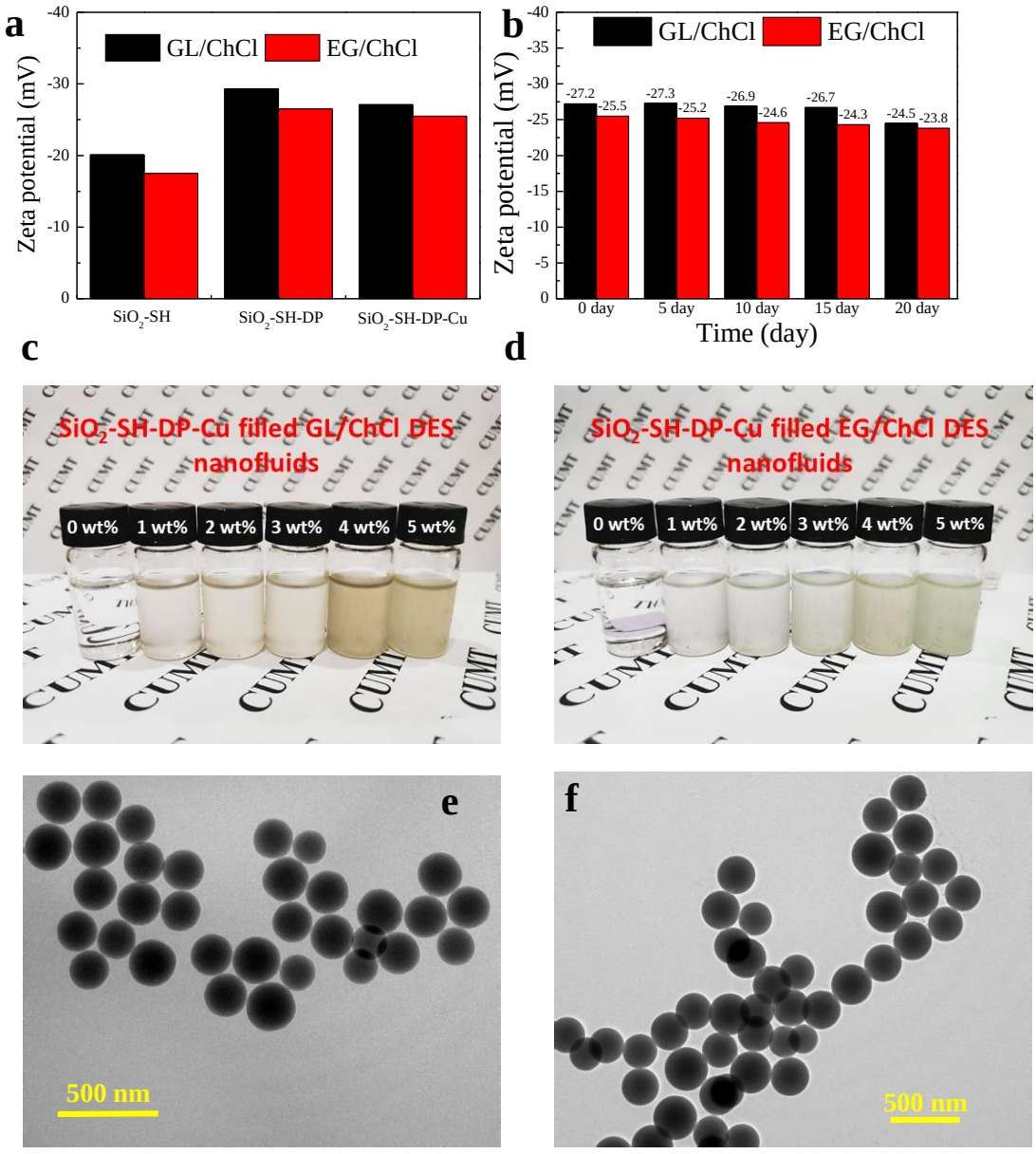


Fig. S2 XPS survey spectra of (a) SiO_2-SH, (b) SiO_2-SH-DP and (c) SiO_2-SH-DP-Cu respectively.

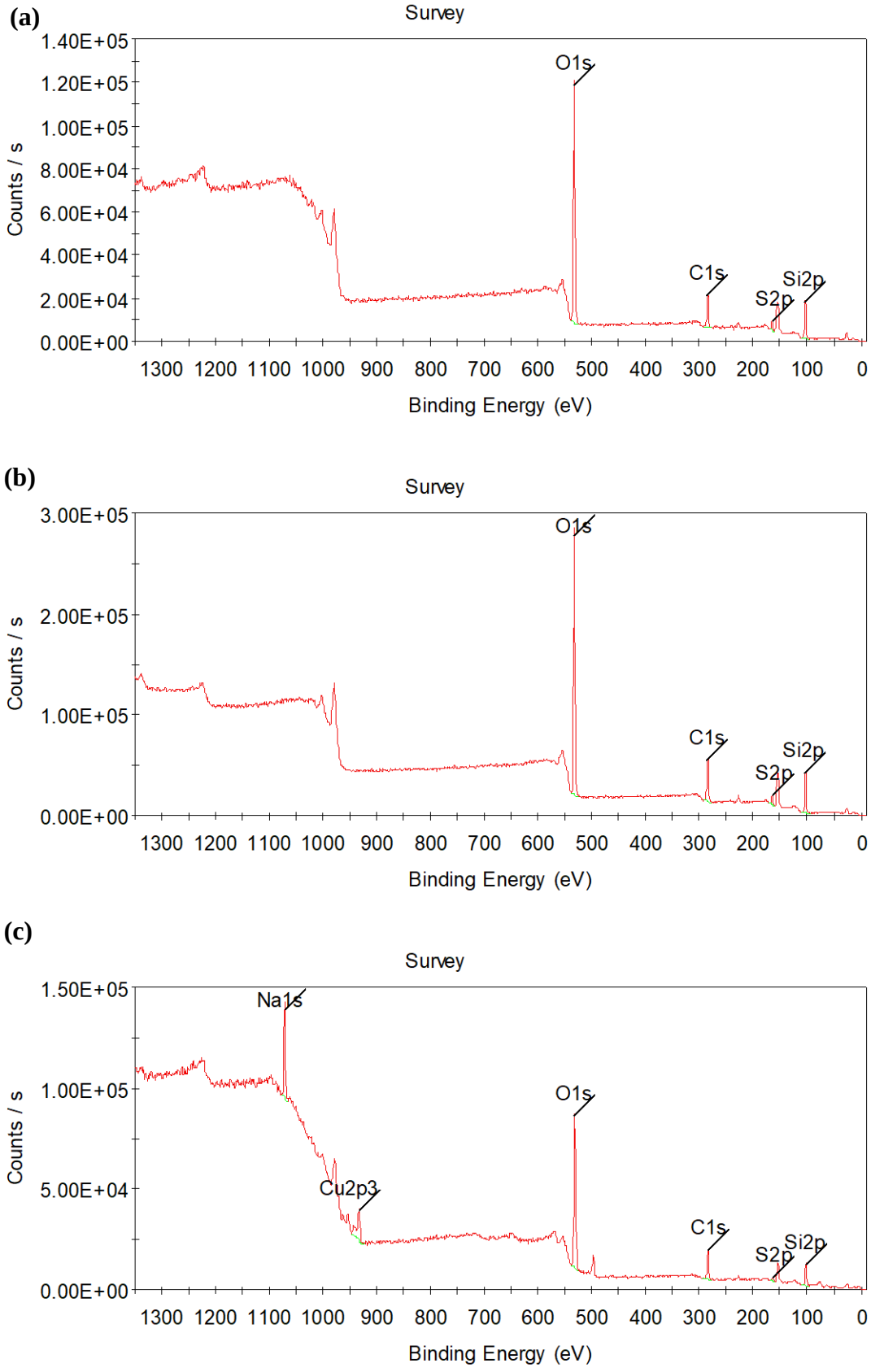
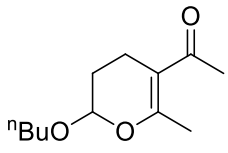
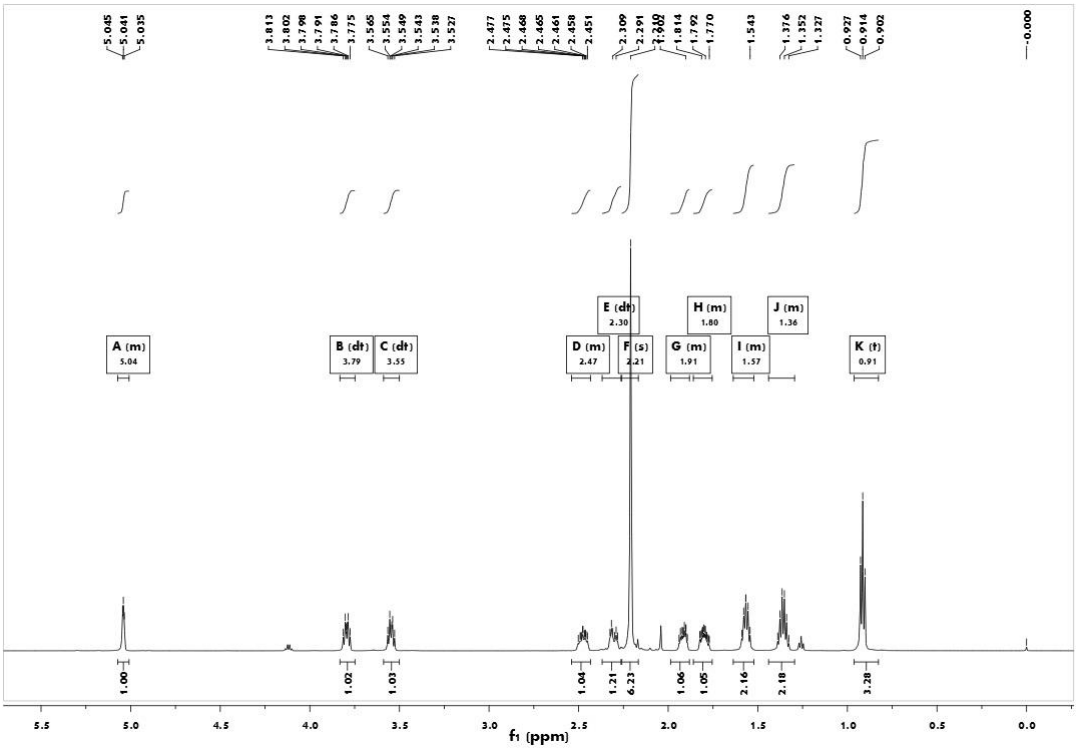
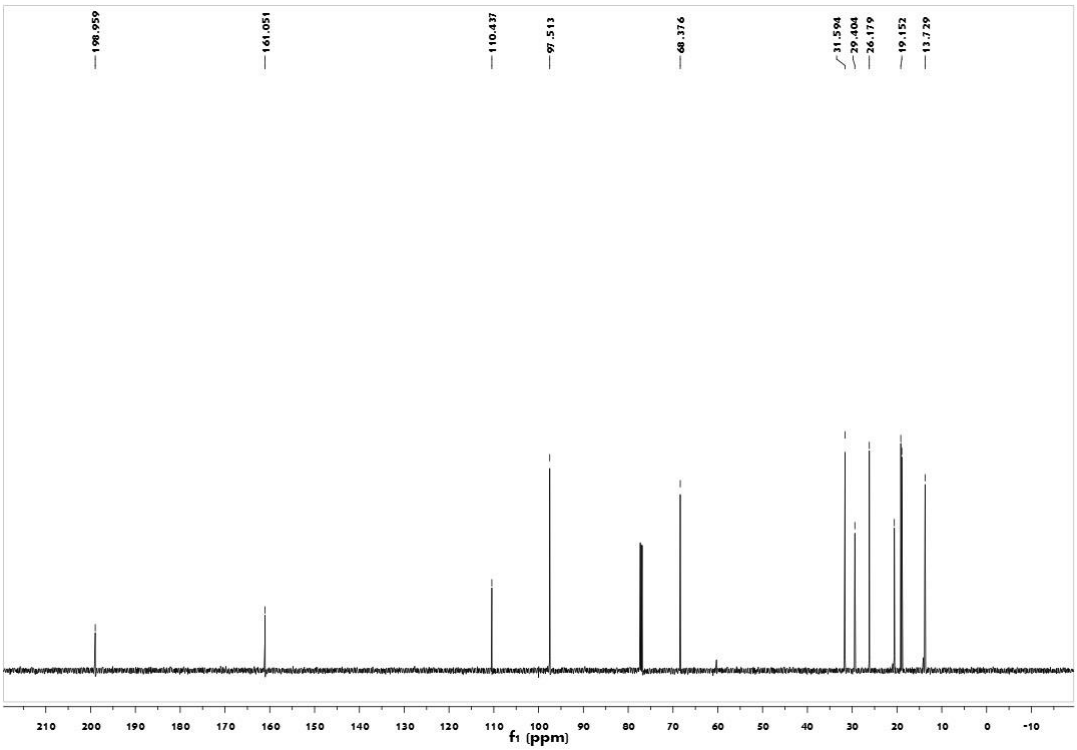


Fig. S3 NMR data and spectra of 1-(2-butoxy-6-methyl-3,4-dihydro-2H-pyran-5-yl)ethanone.



1-(2-Butoxy-6-methyl-3,4-dihydro-2H-pyran-5-yl)ethanone[12]: colourless oil: ^{1}H NMR (600 MHz, $CDCl_3$,25 °C) δ = 5.07 – 5.01 (m, 1H), 3.79 (dt, *J*=9.4, 6.7, 1H), 3.55 (dt, *J*=9.5, 6.6, 1H), 2.54 – 2.43 (m, 1H), 2.30 (dt, *J*=15.9, 4.7, 1H), 2.21 (s, 6H), 1.99 – 1.88 (m, 1H), 1.86 – 1.75 (m, 1H), 1.64 – 1.52 (m, 2H), 1.44 – 1.29 (m, 2H), 0.91 (t, *J*=7.4, 3H).^{13}C NMR (151 MHz, $CDCl_3$,25 °C) δ = 198.96, 161.05, 110.44, 97.51, 68.38, 31.59, 29.40, 26.18, 20.60, 19.15, 18.93, 13.73 ppm.





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