

Supporting Information for
Kust-I: a high-performance two-dimensional graphene-based
material for seawater desalination

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1. The calculations Details of classical molecular dynamics S1

All the molecular dynamics simulations were carried out using the LAMMPS package. The all-atom ClayFF force field was used for Na⁺ and Cl⁻ ions, and the TIP3P water model was adopted for the explicit solvent. For Kust-I, the force field developed by V. Varshney, which has been well documented to reproduce the crystal structure and experimental vibrational spectra, SHAKE constraints were applied to all bonds involving hydrogen atoms. The long-range electrostatic interactions were treated by the Particle Mesh Ewald method, and a typical distance cutoff of 12 Å was used for the van der Waals interactions. The non-bonded interaction pair list was updated every 10 fs. In order to place strain on the Kust-I filter, the cross section along the x-y plane in the simulation box was fixed at a certain value. Canonical sampling was performed through the velocity rescaling method⁵⁷ at constant temperature of 1000 K. An integration time step of 1 fs was used for all simulations. The simulation box contains 4500 water molecules, 245 Na⁺, 245 Cl⁻, a Kust-I filter, and an ideal single graphene sheets used as a piston. The system was firstly equilibrated with z-direction pressure coupling at 1atm for 10 ns, followed by 30 ns productive simulations under a given constant piston pressure in the otherwise NVT ensemble.

2. The calculations Details of the self-cleaning performance S2

Simulation were carried out by Forcite module of commercially available software Materials Studio (Accelrys Software Inc.). Forcite do not support such kind of calculation (Applying an electric field in modelled structures) but it has embedded PERL interpreter. Thus, the procedure of simulation combined with the electric field were carried out by PERL script language. In order to describe interatomic bonds and non-bonding potential energy, the COMPASS (Condensed-phase Optimized Molecular Potentials for Atomic Simulation Studies) force field was used for simulations. Next, the structures were equilibrated by thermostat at desired temperature (300 K) during 100 fs. Such time is required to achieve uniform temperature distribution for the model, time step of simulation was set at 1 fs. The NVT ensemble was used at the next step. From this moment to the end of simulation (till 10 ps) at every time step (1 fs) and the constant value (1 V/Å), electric field strength was added along the electric field direction vector Z component.

3. The POSCAR file of Kust-I

Kust-I

1.0000000000000000

11.5297002792000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.0830001831000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

C

24

Direct

0.0621399999999994	0.9582999920000006	0.5000000000000000
0.0581299970000018	0.7210000239999985	0.5000000000000000
0.1309699970000011	0.5305499910000009	0.5000000000000000
0.0652099980000003	0.3327499789999990	0.5000000000000000
0.1368300050000002	0.1368299980000032	0.5000000000000000
0.2515000080000007	0.2149000080000008	0.5000000000000000
0.2514800120000018	0.4570099920000033	0.5000000000000000
0.3719900059999972	0.5305399960000017	0.5000000000000000
0.4377700169999983	0.3327499789999990	0.5000000000000000
0.3661499849999998	0.1368400019999996	0.5000000000000000
0.4448400039999996	0.7209899899999996	0.5000000000000000
0.4408199929999981	0.9582800029999987	0.5000000000000000
0.5651999740000022	0.6742499949999967	0.5000000000000000
0.6368399819999979	0.8701500259999975	0.5000000000000000
0.7514899999999969	0.7921000239999998	0.5000000000000000
0.7515000080000007	0.5500199660000007	0.5000000000000000
0.6309800260000031	0.4764999949999975	0.5000000000000000
0.5581500039999980	0.2860299929999996	0.5000000000000000
0.5621899909999968	0.0487200000000030	0.5000000000000000
0.9407499750000028	0.0488000009999965	0.5000000000000000

0.9448300370000027	0.2861100080000014	0.5000000000000000
0.8719900059999972	0.4765199839999994	0.5000000000000000
0.9377600079999979	0.6743199960000013	0.5000000000000000
0.8661300090000026	0.8702200270000020	0.5000000000000000

4. Script of the movement of ions in the electric field

```
#!/perl

use strict;

use Getopt::Long;

use MaterialsScript qw(:all);

my $doc = $Documents{"packmol-net-e-gra_nacl.xsd"};

Modules->Forcite->ChangeSettings([

    ElectricFieldStrength => 1,

    ElectricFieldX => 0,

    ElectricFieldY => 0,

    ElectricFieldZ => 1,

    CounterElectricField =>"No"]);

my $results = Modules->Forcite->Dynamics->Run($doc, Settings(

    Quality => 'Medium',

    CurrentForcefield => 'Universal',

    ChargeAssignment => 'Use current',

    Ensemble3D => 'NVT',

    TrajectoryFrequency => 100,

    AssignFixedBonds => 'No'));

my $outTrajectory = $results->Trajectory;

my $results = Modules->Forcite->Dynamics->Run($doc, Settings(

    ChargeAssignment => 'Use current',
```

```
Ensemble0D => 'NVT',  
Ensemble3D => 'NVT',  
Temperature => 300,  
NumberOfSteps => 8000,  
TrajectoryFrequency => 8000));  
my $outTrajectory = $results->Trajectory;
```

5. Synthetic method

The similar two-dimensional carbon structure (Seen the figure below) is constructed with decagonal, hexagonal, and pentagonal carbon rings was synthesized by zeolite template method:

Ultramicroporous Carbon Synthesis Using Lithium-Ion Effect in ZSM-5 Zeolite Template

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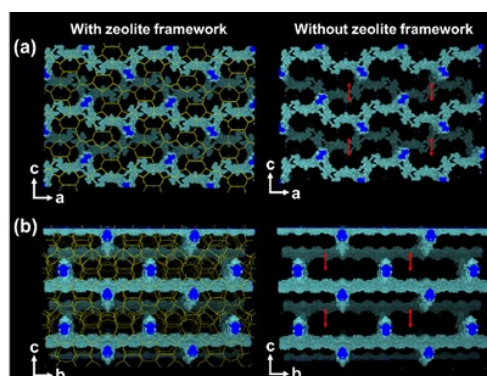
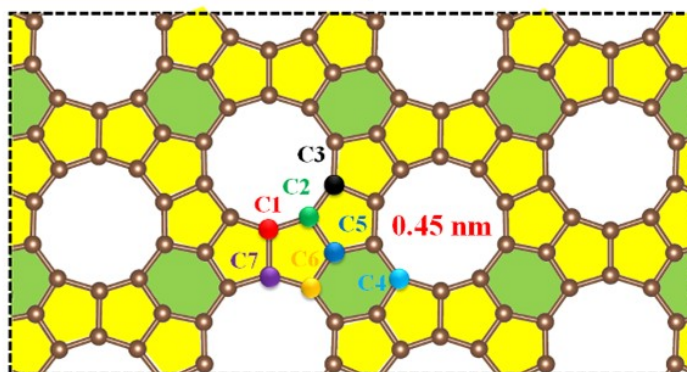
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Supporting Information

ABSTRACT: Zeolite templating is a versatile synthesis route to produce various types of ordered microporous carbon. However, the synthesis thus far has been limited to the use of wide-pore zeolites with 12-membered ring (12MR) pore mouths or more because of the diffusion limitation of organic carbon precursors. Here, we report an extension of the carbon synthesis to a 10MR zeolite, through acetylene carbonization in Li⁺-ion-exchanged ZSM-5 zeolite. The promoting effect of the Li⁺ ions on the carbon synthesis could be relevant to the carbide-forming property of the element, similar to the recently reported cases of La³⁺, Y³⁺, and Ca²⁺ cations in 12MR zeolites. The resultant carbon exhibited an ordered array of ultramicropores of 0.5 nm diameter, which corresponded to the thickness of the zeolite framework. Because of the ultramicroporosity, the ZSM-5-templated carbon exhibited an anomalously high value of surface-area-normalized electrical double-layer capacitance.



Reference

T. Lee, S.H. Ko, S. J. Cho, and R. Ryoo, Ultramicroporous Carbon Synthesis Using Lithium-Ion Effect in ZSM-5 Zeolite Template. *Chem. Mater.*, 2018, 30, 6513-6520).

5.1 Preparation of Zeolite Template

The ZSM-5 zeolite was purchased from Zeolyst (CBV 2314, NH₄⁺ ionic form). For Li⁺-ion exchange, 1 g of zeolite was added to a 32 mL aqueous solution of 0.5 M LiCl. The solution with the zeolite was stirred for 3 h at 60 °C and then filtered. This

treatment was repeated three times in total, to increase the ion-exchange level. Subsequently, the zeolite was washed with distilled water, dried at 100 °C, and calcined at 550 °C in air. The Li/Al molar ratio of the resultant zeolite was 0.8. The Li⁺-ion-exchanged zeolite was designated as LiZSM-5. Calcium-ion exchange was conducted with a 0.5 M CaCl₂ aqueous solution instead of LiCl. The Ca/Al molar ratio of the resultant CaZSM-5 zeolite was 0.4. Both the Zeolyst zeolite and the laboratory-synthesized sample gave the same ion-exchange levels.

5.2 TGA Analysis of Carbon Deposition on Zeolite

The amount of carbon deposition in ZSM-5 zeolite was monitored in situ using a thermogravimetric analyzer (TGA-50, SHIMADZU). The gas flow system of the TGA apparatus was modified to flow a mixture of N₂, acetylene, and H₂O vapor at controlled rates. Typically, 8 mg of zeolite was loaded on a fused-quartz pan. The sample on the pan was slowly heated to 500 °C under a dry N₂ flow of 30 mL min⁻¹. When the temperature reached 500 °C, the N₂ flow was merged with an acetylene gas flow. The combined gas flow was passed through a water bubbler, and the N₂/acetylene/H₂O ratio = 94/2/4 in vol %. The sample weight was monitored over time under this condition.

5.3 Carbon Synthesis

Carbon was synthesized using acetylene as a carbon source and LiZSM-5 (or CaZSM-5) as a template. In a typical synthesis, 0.2 g of LiZSM-5 was loaded in a vertical plug-flow fused-quartz reactor, which was equipped with a fritted quartz disk. The reactor temperature was increased to 500 °C and maintained there for a given

time under a N₂–acetylene–H₂O mixed gas flow of 94/2/4 vol % composition, as in the TGA experiment, except that the total flow rate was 50 mL min⁻¹. The gas flow was then switched to dry N₂. Subsequently, the reactor temperature was increased to 900 °C and maintained there for 2 h before cooling to room temperature. The resultant carbon/zeolite composite was slurried in a 0.3M HF/0.15M HCl solution to release the carbon product from the template. The carbon was filtered, washed with distilled water, and dried in an oven at 100 °C.

The final product is as follows:

