Article

Synthesis of Graphene Quantum Dots Enhanced Nano $Ca(OH)_2$ from ammoniated $CaCl_2$

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Supplementary Material

3.1 Morphology and Particle Size Distribution

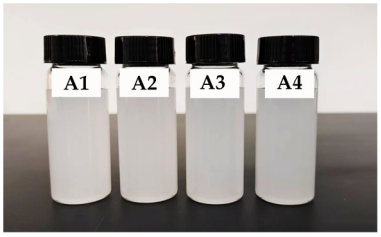


Figure S1. Photograph of prepared samples

3.4. First-Principle Calculations of the Reaction and Combination

Table S1. Ground-state energy and the Energy contribution of each chemical in Equation (5)

Chemicals	Ground-state energy (eV)	Energy contribution in reaction (eV)
$CaCl_2$	−25.62	−51.25
$NH_3{\cdot}H_2O$	−34.05	−1089.68
$CaCl_2{\cdot}(NH_3)_8$	−686.78	−686.78
H_2O	−14.32	−458.15

Table S2. Ground-state energy and the Energy contribution of each chemical in Equation (6)

Chemicals	Ground-state energy (eV)	Energy contribution in reaction (eV)
$CaCl_2{\cdot}(NH_3)_8$	−686.78	−686.78
NaOH	−27.28	−109.12
H_2O	−14.32	−458.15
$Ca(OH)_2$	−28.65	−57.30
NaCl	−27.11	−108.45
$NH_3{\cdot}H_2O$	−34.05	−1089.68

Table S3. Ground-state energy of each chemical for binding energy calculation in Equation (8)

Chemicals	Ground-state energy (eV)
GQDs	−596.31
$Ca(OH)_2$-(001)	−1367.02
$Ca(OH)_2$/GQDs	−1964.24