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1 **Precipitated Calcium Hydroxide Morphology in Nanoparticle Suspensions: An** 2 **experimental and molecular dynamics study**

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12 **Abstract:** The volume and morphology of calcium hydroxide (CH) precipitating from supersaturated solutions is
13 monitored as a function of the concentration of either of two types of nanoparticles dispersed in the solution. The
14 CH precipitated in the presence of sulfonated graphene nanosheets (SGN) had well-developed hexagonal platelet
15 shapes, while that forming in the presence of cationic polyurethane nanospheres (PUC) tended to aggregate around
16 the PUC and developed as spherulitic masses. The terminal CH platelet size in SGN suspensions was 8 μm ; with
17 increasing SGN dosage, the mean size increased to 23 μm . Taking into consideration complementary experimental
18 measurements of isothermal adsorption and zeta potential, we speculate that calcium from the solution adsorbs on
19 the surfaces of both SGN and PUC prior to nucleation of CH. Furthermore, molecular-scale mechanism indicated
20 the interaction of Ca-Ocoo from PUC is stronger than Ca-Oso₃ from SGN. Simultaneously the number of adsorbed
21 calcium by PUC is roughly 3 times greater than for SGN, which is perfectly matched with the measured adsorption
22 isotherm. Hopefully, this work can provide scientific guidance for hydration mechanism of cementitious materials in
23 the presence of nanoparticles suspensions.

24 **Keywords:** Calcium Hydroxide; Nanoparticle suspensions; Molecular dynamics;

25 **1 Introduction**

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