Molecular dynamics simulations of peptoids adsorbed onto calcite surfaces: Which molecule-surface interactions alter calcite growth rates?

MALINI R. INNOCENTI, SHAUN A. HALL[1*] AND
JOHN H. HARDING[2]

[1]Department of Materials Science and Engineering Sir Robert Hadfield Building, Sheffield, S1 3JD, UK
shaun.hall@sheffield.ac.uk
[2]Ibid, j.harding@sheffield.ac.uk

Peptoids, or poly N-substituted glycines, are biomimetic compounds for proteins that can be altered by very simple chemistry involving substitutions at the nitrogen and contain less complexity due to their lack of the normally chiral alpha-carbon present in peptides. These molecules are very useful as models in experiments studying the effect of the physical and chemical structure of peptides on mineral growth (in the biomineralisation of calcite in aquatic species such as coccolithophores). They are also of interest in promoting the sequestration of carbon dioxide from the atmosphere as calcite. Experimental work[1] found that peptoids of similar molecular weight had significantly different effects upon the growth and morphology of calcite based on their differences in acidity, connectivity and substitution patterns. By studying the adsorption of a set of these molecules to flat, stepped, and kinked calcite surfaces using molecular dynamics simulations, it was determined that no single thermodynamic or structural parameter was capable of identifying the peptoid species that were associated with calcite growth enhancement. It was, however, determined that a combination of binding energy, radius of gyration, and the variation in the radius of gyration at the surface of calcite was able to clearly identify peptoids capable of increased calcite growth. This metric was then further tested against a second set of peptoid molecules, when it identified again the best potential peptoid species for enhancing calcite growth, indicating its potential use in a screening method for computationally identifying useful calcite growth enhancers based on peptoid architectures.

[1] Chen *et al.* (2011), *J. Am. Chem. Soc.* **2011**, 133, 5214-7