Molecular simulations of succinate adsorption at steps on calcite {104}

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We report Molecular Dynamics (MD) simulation results for succinate and Na^+ adsorption at steps on calcite {104} in water. Surface inter-atomic distances (Ca-$O_{CO3,i}$) are elongated compared to water alone, suggesting easier surface Ca^{2+} detachment, consistent with observed increase in dissolution rate. Succinate adsorption lowers step energies, which explains the appearance of steps in unusual directions as observed by atomic force microscopy. Finally, the adsorption affinity sequence at different steps is related to step-appearance sequence (i.e., velocity), suggesting that Ca^{2+} removal is blocked by succinate, thus, controlling the directions of etch-pit dissolution and, hence, pit morphology. Our study provides a strong example of the utility of MD simulations, when closely linked to experimental results, in understanding the formation of unusual biomineral crystal morphologies that may serve as biosignatures on Earth and, potentially, on other worlds.

The magmatic response to Indo-Asia collision in southern Tibet

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Indo-Asia collision is one of the great tectonic events with global significance in the Earth's history. The timing of the initiation of the collision, however, is still a matter in dispute. Multiple evidences in southern Tibet support that the Indian–Asian collision proceeded from a "soft" phase at ~ 65–70 Ma to a "hard" phase at ~ 45–40Ma, followed by continued post-collisional convergence to the present [1,2,3]. The most attract is an ca.1500 km- extending giant unconformity between the horizontal terrestrial Paleogene strata and the underlying strongly- deformed submarine upper Cretaceous- Permian strata. The overlying strata, the Lizizong volcanic succession (LVS) are >5 km in thickness and formed during the period of 70- 40 Ma [4], showing the signatures from subductional to collisional- postcollisional upwards. Ages from 69.97 Ma to 58.64 Ma for the bottom of the LVS along the strike of the unconformity have been determined by zircon SHRIMP U-Pb dating and $^{40}Ar/^{39}Ar$ dating, implying the diachroneity of the initiate timing of the Indo-Asia collision. Both the syn-collisional LVS and granitic batholiths (with a peak age of ~ 50Ma) formed the majority of the Gangdese magmatic belt. Similar to the LVS, these batholiths also show positive values of εNd (t) and zircon ε_{Hf} (t) (+2.34–+8.26, +6.3 – +14.7, respectively) and contain abundant mafic microgranular enclaves (MME) and associated mafic intrusions, indicating significant mantle contributions to crustal growth in southern Tibetan[5]. The post-collisional igneous rocks are of a wide variety and their distribution defines a distinctive pattern of migration with time, implying the heterogeneity of the magma sources and possible lateral flow of the lower crust and/or the asthenospheric mantle induced by the collision[6].

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