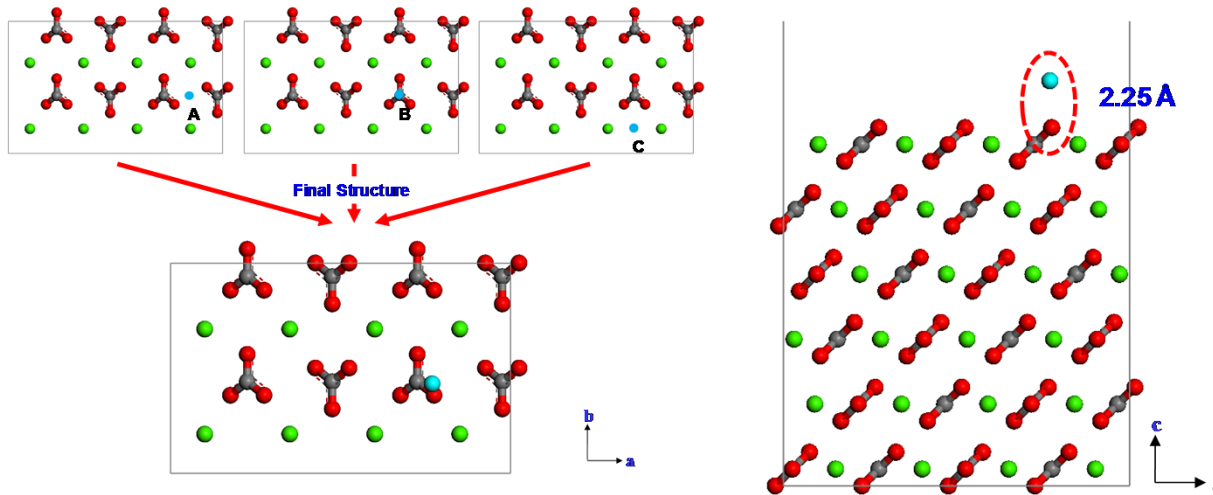


# Adsorption of Calcium ion and Benzolates on Calcite ( $10\bar{1}4$ ) Surface

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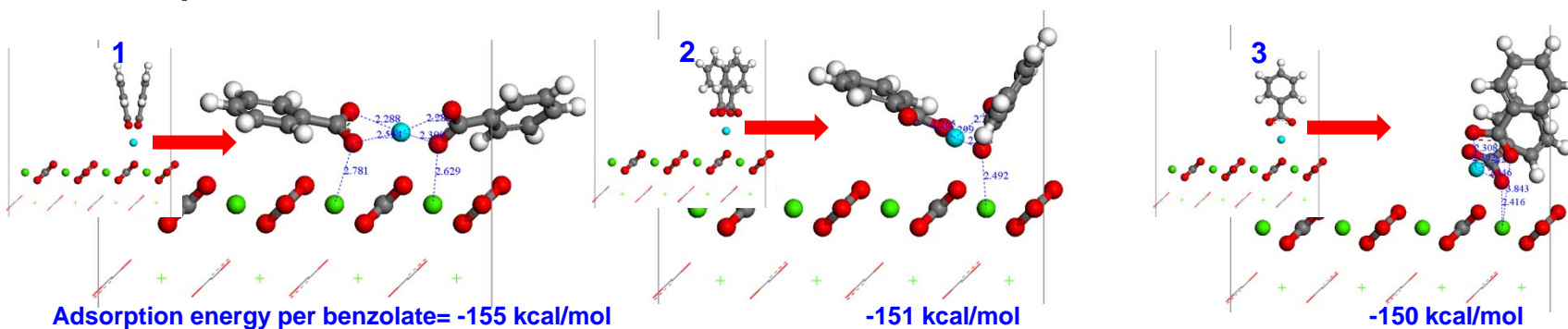
## Adsorption of calcium ion on the calcite slab surface:



To investigate the adsorption configuration of calcium ion on the calcite slab surface, we set 3 different initial positions (A, B or C) for calcium ion. We found that final structures after geometry optimization using DFT are same. We expect that the position of calcium ion on the final structure is most stable adsorption position with calcite slab surface.

**Adsorption energy = -71 kcal/mol**

## Adsorption of benzolates on the calcite slab surface:



Each oxygen on benzolate interacts with the adsorbed calcium ion as well as the closest calcium atom on the first layer of calcite slab surface. However, we found that the adsorption energy is not significantly depended on the initial positions (1, 2 or 3) of benzolates.