Séminaire de Chimie Théorique

Salle réunion THEO, 3eme Est, bat. A12

Lundi 09 Février à 11:00

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Silicon surfaces: fragmentation methods and thermal simulations

One method to calculate the properties of non-conducting crystals is systematic molecular fragmentation (SMF). This can equally be applied to crystal surfaces and adsorbate-surface interactions. In this talk I shall describe SMF in general, its application to H + H-Si(111), and recent progress toward including surface temperature effects.

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