Ab initio molecular dynamics simulations of Ti2 on C 20 collisions and C20Ti2 configurations

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The dynamics of the collision process of a titanium dimer against a C 20 nanocluster in the bowl configuration is simulated by means ab initio molecular dynamics, focusing our interest on the first steps to synthesize Ti2C20 clusters, characterizing the relevant structures generated during the collision process. The electronic localization function is also calculated. The early stages of the dynamics are critical to determine the outcome because of the large kinetic energy of the Ti dimer, which allows it to wander around the C20 cluster.