Theoretical Study of the Structure and Electronic Properties of Si 3O n -and Si 6O n -(n=1-6) Clusters. Fragmentation and Formation Patterns

Tiznado, William

Oña, Ofelia B.

Caputo, María C.

Ferraro, Marta B.

Fuentealba, Patricio

A theoretical study of two series of small clusters, Si 3O n-and Si 6O n -(n=1-6), has been carried out. The minimum energy structures were produced adding an electron to neutral species followed by relaxation at the B3LYP-6-311G(2d) level. The vertical ionization energies (VIEs) were computed using the electron propagator theory (EPT) in two approximations, Unrestricted Outer Valence Green Functions (UOVGF) and partial third-order approximation (P3). In the series Si 3O n -the theoretical VIEs of the minimum energy structures agree well with experimental data. For the second series there are not experimental VIEs, and the theoretical results are predictions. The performance of EPT methodologies in conjunction with all-electron or pseudopotentials (PP) calculations is analyzed. The conjunction of P3 and PP approximation proves to be the most efficient and economical methodology to calculate the VIEs of small anionic silicon oxide clusters. In the series Si 6O n -different channels of f