



FIG. 2 Initial (*left*: top view; and *middle*: side view) and final (*right*: top view) configurations of the simulated complexes; (A) C1, (B) C2, (C) C3, and (D) C4. siRNAs are given in cyan, 568 Da PEIs are in gray, and 1874 Da PEIs are in orange. Water and ions are removed for clarity [61].

gradually encapsulated in the CST/CS nanogel through the hydrophobic interactions of the nanogel hydrophobic domains and the FSH hydrophobic patch (Fig. 10). The FSH flexibility decreased when the nanogel was added except for its hydrophobic patch domain. Therefore the FSH-nanogel interactions could be investigated by such molecular level simulations to design ideal CST/CS nanogels as the protein carriers.

3. GRAPHENE AND ITS DERIVATIVES AS DRUG DELIVERY SYSTEMS

When graphene was prepared in 2004, it found numerous applications as it illustrated incredible low toxicity, biocompatibility, biodegradability as well as electronic and structural properties [27, 28]. Graphene is a material of one atom thickness thus it has been used in various applications including drug carriers, chemical and