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Mechanism of Cationic Nanoparticles and Cell-Penetrating Peptides Direct Translocate Across Cell Membranes JIAQI LIN, ALFREDO ALEXANDER-KATZ, Massachusetts Inst of Tech-MIT — Cationic Nanoparticles (NPs) and cell-penetrating peptides (CPPs) are known effective intracellular delivery agents. These positively charged particles can bypass traditional endocytosis route to enter the cytosol, which is known as direct translocation. However, mechanism of direct translocation of both NPs and CPPs is not well understood. Using Coarse-grained (CG) molecular dynamics simulation, we found that gold nanoparticles (AuNPs) as well as HIV-1 Tat peptides can translocate across model biological membranes through nanoscale holes under a transmembrane (TM) potential. After the translocation, the TM is strongly weakened and the holes gradually reseal themselves, while the NPs/CPPs roam freely in the "intracellular region." Both size and shape of the NPs/ CPPs are found to be a determine factor of their translocation behaviour, and the relationship between direct translocation and endocytosis is also discussed. The results provided here establish fundamental rules of direct translocation entry of NPs/CPPs, which may guide the rational design of cationic intracellular nanocarriers.

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