Molecular aspects of core-shell intrinsic defect induced enhanced antibacterial activity of ZnO nanocrystals

Por: Verma, SK (Verma, Suresh K.)[1]; Jha, E (Jha, Ealisha)[2]; Panda, PK (Panda, Pritam Kumar)[1]; Das, JK(Das, Jugal K.)[1]; Thirumurugan, A (Thirumurugan, Arun)[3]; Suar, M (Suar, Mrutyunjay)[1]; Parashar, SKS(Parashar, S. K. S.)[4]
Ver ResearcherID y ORCID

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Resumen

Aim: To investigate molecular aspects of the antibacterial effect of size-dependent core-shell intrinsic defects of nanocrystalline ZnO synthesized through high energy ball milling technique. Materials & methods: Mechanically synthesized and characterized 7, 10 and 15 h milled ZnO nanoparticles were evaluated for antibacterial activity with molecular investigation by computational molecular docking. Results: Synthesized ZnO nanoparticles displayed shrinkage of core and increase of shell with reduction in size of bulk ZnO particles from 250 to 80, 40 and 20 nm and increase in zeta potential up to -19 mV in 7, 10 and 15 h nano ZnO. Antibacterial activity was found increased with decrease in size due to increased reactive oxygen species andmembrane damage in bacteria. Conclusion: Synthesized nano ZnO exhibit size-dependent antibacterial action as consequences of interactions with cell membrane proteins via hydrogen bond interaction with amino acid residues followed by internalization, membrane depolarization and induction of reactive oxygen species generation.

Palabras clave

Palabras clave de autor:antibacterial activity; core-shell model; cytotoxicity; high energy ball milling (HEBM); membrane potential; membrane protein; molecular docking; nano ZnO; oxygen vacancies; ROS
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Información del autor

Dirección para petición de copias: Parashar, SKS (autor para petición de copias)

+ KIIT Univ, Sch Appl Sci, Bhubaneswar 751024, Orissa, India.

Direcciones:

+ [1] KIIT Univ, Sch Biotechnol, Bhubaneswar 751024, Orissa, India
+ [2] Mem Univ Newfoundland, Dept Phys & Phys Oceanog, St John, NF A1C 5S7, Canada
+ [3] Univ Chile, Fac Math & Phys Sci, Dept Mech Engn, Adv Mat Lab, Santiago, Chile
+ [4] KIIT Univ, Sch Appl Sci, Bhubaneswar 751024, Orissa, India

Direcciones de correo electrónico:sksparashar@yahoo.com

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FUTURE MEDICINE LTD, UNITEC HOUSE, 3RD FLOOR, 2 ALBERT PLACE, FINCHLEY CENTRAL, LONDON, N3 1QB, ENGLAND

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