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In silico energy paradigms studies towards stability of nano-encapsulated piperine alkaloid for delivery to Alzheimer's disease plaque sites in mouse brain

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The molecular modeling and, energy studies conclusively showed that the initial piperine energy (27.2 KJ/Mol) at its minimum energy conformation was changed to 9.7 KJ/Mol with addition of single water molecule (piperine+H_2O) which further goes down to -21.8 kJ/mol (piperine+2H_2O), and -48.6 kJ/mol (piperine+3H_2O) indicating a stabilization pattern for the piperine molecule. The net addition of one molecule each of glycerol mono-stearate (GMS) and benzyl alcohol (BA) along with 3 molecules of water and, one molecule of piperine put the conformationally stabilized minimum energy status at 28.3 KJ/Mol, further indicating a stabilized matrix for this constitution. A closer look at energy paradigm with the appropriated ratios of the BA and, GMS as well as water molecule(s) showed an energy levels for the piperine+BA to be at 73.4 kJ/mol which is exactly in the range for the energy status of the BA itself at 76.7 KJ/Mol in its minimum energy conformation status and, thus providing not only much effective change for the BA+piperine system as well as the piperine being considered as dormant (not significantly contributing to the net energy change of the system). Although the system itself is now at moderate energy levels, a further water addition puts it back to 21.3 KJ/Mol (piperine+H_2O+BA). Addition of more water molecules (3H_2O), one molecule of GMS hardly changes the energy levels of the composition which now stands at 28.3 KJ/Mol, stable enough for delivery, storage and distribution in the intended tissue as compared to the initial energy states. The chemically higher energy status piperine molecule now rests as part of the stabilized composition. Surprisingly, the higher energy status of one GMS molecule at 121.7 KJ/ Mol in the composition (piperine+GMS+BA+3H_2O) stands as at 28.3 KJ/Mol and, thereby comfortably being part of the stabilized matrix for the developing nano matrix. The energy paradigms also suggested the careful ratio of the constituents, the piperine, lipid part GMS and, some BA as well as, of course water which is major constituent. Moreover, the increase in the ratios of BA and, GMS in relation to water where piperine ratio is fixed at initial level will change the energy status to higher order and, destabilize the matrix. For biological interaction and, transport conditions, there are changes in the energy status depending upon the surface interactions of the incoming chemical entity and, this phenomenon either further stabilize the matrix or, tend it to erode or, for that matter react in a suitable way according to the energy conditions prevailing. However, the energy in the core will remain in the stabilization range till the erosion/burst or, other destabilization forms take place with the matrix, i. e. nano-carrier. The prepared piperine-lipid-nanoparticles (PSLN) were found to be stable and, deliverable to mouse brain tissues with good amount of payload delivery capabilities as observed experimentally. The uncoated PSLN has shown a good antidepressant action via increase in duration of action of piperine at an equivalent 20 mg/kg dose whereas PS-80 coated PSLN have showed effective anti-Alzheimer's action via maximum clearance of β-Amyloid plaques as compared to the naked piperine or, uncoated PSLN. The prepared Solid Lipid Nanoparticles (SLN) was also suitable as preferred nano-carrier for preparations requiring lipophilic conditions and, other lipophilic drugs. The prepared SLN are also capable of delivering short-half life drugs, phyto-constituent and, light and air-sensitive product as well.

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Stretchable transparent composite conductors and elastomeric thin film electronics

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We have developed a new transparent composite electrode technology that can match the transparency and sheet resistance of indium tin oxide, and the mechanical flexibility of polymers. When a rubbery polymer was selected for the matrix, the transparent composite electrode can be stretched by greater than 100% strain repeatedly without much loss of surface conductivity. Stretchable thin film devices, including dielectric elastomer actuators and light emitting diodes have been fabricated based on the elastomeric transparent conductors. The materials selection and device architecture that lead to highly flexible and stretchable polymer OLEDs will be reported. The OLEDs can be reversibly stretched by up to 50% strain, twisted, and folded.

Biography

Qibing Pei received a B.S. in chemistry from Nanjing University, China, and a Ph.D. from the Institute of Chemistry, Chinese Academy of Science, Beijing. He was a postdoctoral fellow during 1991-1993 at Linköping University, Sweden, 1993-1994 at UNIAX Corporation (now DuPont Display), Santa Barbara, and a staff chemist of UNIAX during 1994-1997. He worked as senior chemist at Imation Corporation, St Paul, MN (1997-1998) and a senior research engineer at SRI International, Menlo Park, CA (1998-2004). He has been a Professor of Materials Science and Engineering, UCLA, since 2004. He was named a Fellow of the SPIE in 2012.

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