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"ALD and related ultra-thin film processes foradvanced devices"

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Aggregation problem of dye monolayer in dye sensitized solar cells

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Dye sensitized solar cells are photovoltaic devices which simulate photosynthesis [1,2]. Comparing to other solar cells, they cost less and are easy to manufacture. One of themost important parts of this system is adye. A monolayer of dye, adsorbed onto semiconductor surface collects sunlight, which is further being transformed into electrical energy.

Many types of sensitizers are known today: organic, inorganic, synthetic, natural[3].Cells with synthetic ruthenium dyes have the highest efficiency of conversion sun energy into electrical. The greatdisadvantage of ruthenium dyes is their price. Natural pigments, on the other hand, extracted from plants, fruits andflowers are available and affordable, though they gain efficiency of conversion of only a fewpercent. The basic problem with using natural dyes as sensitizers is their aggregation on the semisonductor surface.

A major factor responsable for the low phtoconversion efficiencyof an organic dye sensitized solar cell is the formation of dye aggregate on the semiconducuctor surface. Such an aggregation effect can bring about significant changes in the absorption and photosensitizing properties of the sensitizing dye molecule. One can minimize aggregation effect on the semiconductor surface using dyes with particularanchoring groups[4] or antiaggregation coadsorbents[5]. Computational calculations (density functional theory(DFT), time-dependent DFT (TDDFT))are also a convenient approach for investigation of aggregationof dye molecules [6].

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