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### Diamond surface modification for biomolecule interactions in the design of medical implants

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**A**vascular necrosis is a disease of cell death in joints, jaw, and hips due to lack of blood supply induced by burnt, inflammation or trauma, etc. The mainstream curing these days are i) arterial infusion by partial drug delivery, and ii) the replacement of the whole joints by using artificial materials. The first method can only be applied at an early stage of the disease, and the curing results. So for more severe situations, the medical implants will become the only choice. With the need for an improved stability and biocompatibility of the medical implant materials, diamond has recently become interesting as a promising material. The combination of chemical inertness and biocompatibility makes diamond a good material for e.g. biological applications. In order to promote localized cell adhesion and vascularization onto the diamond-covered medical implants, the prerequisite for pre-adhesion of growth factors onto the diamond surfaces is of largest interest to study more in detail. It is highly necessary that these

investigations are performed on an atomic level. Therefore, theoretical simulations are a necessary complementary tool to i) aid in the analysis of experimental observations, and ii) to make recommendations for corresponding experimental studies. With the purpose to tailor-make the medical implant surface by utilizing diamond's unique properties, the present study has investigated the interaction between diamond and various biomolecules (BMP2, RGD, heparin, fibronectin, VEGF, angiopoietin). The combined effect of various surface plane and termination type (H, O, OH, and NH<sub>2</sub>) has been of a special interest to study. Three different groupings were obtained with regard to adhesion strength. And all of these three groups showed different dependencies of the surface termination type. For all of these different scenarios, strong bond formations were observed. Evaluation of the methods used showed that the calculated trends in adhesion energy are highly reliable.

#### Biography

Karin Larsson is a Professor in Inorganic Chemistry at the Department of Materials Chemistry, Uppsala University, Sweden. She received a PhD in Chemistry (especially Inorganic Chemistry) in 1988 at the Department of Chemistry, Uppsala University. The research was directed towards investigation of molecular dynamic processes in solid hydrates by using solid state NMR spectroscopy. The Post-Doctoral period 1989-1990 was devoted to diamond growth using different CVD setups. Since autumn, 1991, and onwards Prof. Larsson continued to theoretically investigate surface processes during. Prof. Karin Larsson is today the leader of the Theoretical Materials Chemistry Group at the Department of Chemistry. The scientific focus is on interpretation, understanding and prediction of the following processes/properties for both solid/gas interfaces, as well as for solid/liquid interfaces; i) CVD growth, iii) interfacial processes for renewable energy applications, and iv) interfacial processes for e.g. bone regeneration (incl. biofunctionalisation of surfaces).

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