

Supporting Information

for

Detonation nanodiamonds biofunctionalization and immobilization to titanium alloy surfaces as first steps towards medical application

Juliana P.L. Gonçalves^{§,1}, Afnan Q. Shaikh^{§,1,2}, Manuela Reitzig¹, Daria A. Kovalenko^{1,2}, Jan Michael^{1,3}, René Beutner², Gianaurelio Cuniberti², Dieter Scharnweber² and Jörg Opitz*,^{1,2}

Address: ¹Inspection and Diagnosis Methods, Fraunhofer Institute for Ceramic Technologies and Systems –Materials Diagnostics, Maria-Reiche-Str. 2, 01109 Dresden, Germany; ²Max Bergmann Center of Biomaterials MBC, Technische Universität Dresden, Budapest Str. 27, 01069 Dresden, Germany and ³Chair of General Biochemistry, Technische Universität Dresden, Bergstr. 66, 01069 Dresden

Email: Dr. Jörg Opitz - joerg.opitz@ikts-md.fraunhofer.de

* Corresponding author

§both authors contributed equally

Physisorption Test

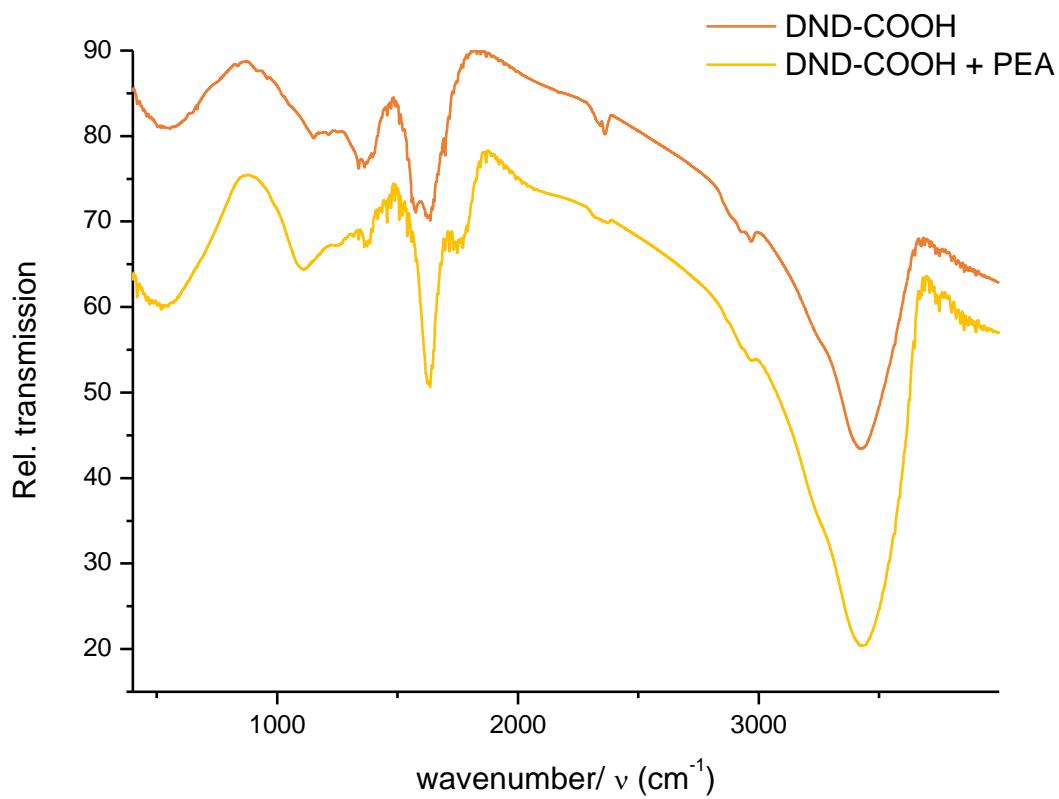


Figure S1: Physisorption test was carried out on carboxylic DND with O-PEA: An aqueous solution (10 mL) of 200 mg carboxilated DND **2** was allowed to react with O-PEA (8% aqueous solution) for 2.5 h, at room temperature. Both products were compared by FTIR. After the incubation time there is no signal form the O-PEA in the final product, indicating that no physisorption occurred.

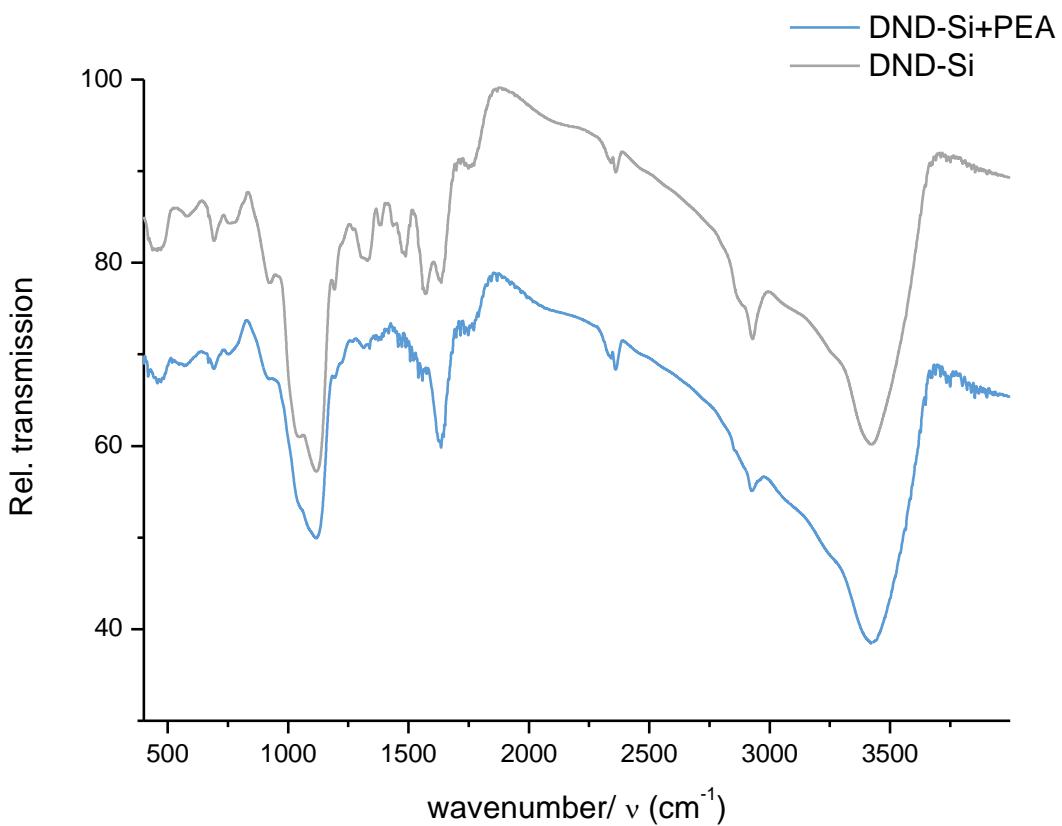


Figure S2: Physisorption test was carried out on silanized DND with O-PEA: An dichloromethane solution of 200 mg of silanized DND **5** and 80 mg of O-PEA, was allowed to react for 65 h, at room temperature. Both products were compared by FTIR. After the incubation time there is no signal from the O-PEA in the final product, indicating that no physisorption occurred.

Table S1: Characteristic absorption bands of species analyzed by infrared spectroscopy, Figure 2 and 3 [1,2].

DND 1	DND-COOH 2	DND-CO-PEA 3	DND-OH 4	DND-APTMS 5	DND-APTMS-PEA 6	O-PEA	Characteristic absorption
		515 cm ⁻¹			535 cm ⁻¹	525 cm ⁻¹	
				690 cm ⁻¹	570 cm ⁻¹	565 cm ⁻¹	
		750 cm ⁻¹			775 cm ⁻¹	760 cm ⁻¹	
		930 cm ⁻¹		925 cm ⁻¹	940 cm ⁻¹	943 cm ⁻¹	δ_{NH_2}
		1030 cm ⁻¹		1050 cm ⁻¹	1025 cm ⁻¹	1025 cm ⁻¹	Si-OR
		1106			1100 cm ⁻¹	1085 cm ⁻¹	Phosphate
1110 cm ⁻¹	1150 cm ⁻¹	1070	1170 - 1120 cm ⁻¹	1120 cm ⁻¹	1150 cm ⁻¹	1155 cm ⁻¹	$\nu_{\text{C}-\text{O}}$
1220 cm ⁻¹			1210 cm ⁻¹		1250 cm ⁻¹	1250 cm ⁻¹	
	1340 cm ⁻¹		1370 cm ⁻¹	1320 cm ⁻¹			$\delta_{\text{C}-\text{O},\text{H}}$
	1570 cm	1500 cm ⁻¹		1480 cm ⁻¹	1560 cm ⁻¹	1556 cm ⁻¹	NH ₂ scissoring
1620 cm ⁻¹	1630 cm ⁻¹		1630 cm ⁻¹	1638 cm ⁻¹	1638 cm ⁻¹	1630 cm ⁻¹	$\nu_{\text{C}=\text{O}}$
1735 cm ⁻¹			1755 cm ⁻¹			2110 cm ⁻¹	O-H stretching
					2640 cm ⁻¹	2640 cm ⁻¹	ν_{Alkanes}
					2694 cm ⁻¹	2900 cm ⁻¹	
2934 cm ⁻¹	2970 cm ⁻¹	2930 cm ⁻¹	2920 cm ⁻¹	2930 cm ⁻¹	2910 cm ⁻¹	2990 cm ⁻¹	
3415 cm ⁻¹	3420 cm ⁻¹		3410 cm ⁻¹	3420 cm ⁻¹	3430 cm ⁻¹		OH

References

1. Coates, Interpretation of Infrared Spectra, A Practical Approach. In: *J. Encycl. Anal. Chem.*, Ed, John Wiley & Sons: Chichester, 2000
2. Gong, W. *Int. J. Miner. Process.* **2001**, 63, 147–165.