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Supporting information

for

2-D ORGANIZATION OF SILICA NANOPARTICLES ON GOLD SURFACES: CO₂ MARKER DETECTION AND STORAGE

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A- General Methods

PASC-CO₂ adsorption process: The experimental set-up for the CO₂ adsorption experiments was performed inside the Planetary Atmospheres and Surfaces Chamber (PASC), a dedicated planetary simulation chamber (Fig. S1).



Fig.S1. Schematic drawing of the planetary environmental simulation chamber

XPS analysis: The XPS measurements of the samples were recorded before and after the exposure to CO₂ atmosphere inside PASC. The XPS analysis of the samples was carried out in an ultrahigh vacuum chamber equipped with a hemispherical electron analyzer and with the use of an Al K α X-ray source (1486.6 eV) with an aperture of 7 mm × 20 mm. The base pressure in the chamber was 5 × 10^{-10} mbar, and the experiments were performed at room temperature. The peak decomposition in different components was shaped, after background subtraction, as a convolution of Lorenztian and Gaussian curves. Binding energies were calibrated against the binding energy of the Au 4f_{7/2} peak at 84.0 eV for the gold samples. We have not observed any beam radiation damage of the silicon nanoparticles on gold surface during the data acquisition.

IR analysis: Fourier-transform infrared (FTIR) spectroscopy of the Au_SiO₂ samples were performed in a Thermo-Scientific-Nicolet spectrometer. Spectra (2 cm⁻¹ of resolution and 128 scans) were collected in the mid-infrared region (400–4000 cm⁻¹), using a DTGS-ATR detector and a XT-KBr beamsplitter.

SEM microscopy (images and spectra): A field emission scanning microscope (FE-SEM) ThermoScientific APREO C-LV equipped with an energy-dispersive X ray microanalysis system (EDX) Aztec Oxford.

AFM microscopy: Surface morphology was measured by atomic force microscopy (AFM) using an XE-150 SPM / AFM (Park Systems Corp., Suwon, Korea), operating in air at room temperature. True Non-Contact ModeTM provided high-resolution images of SiO₂ nanoparticles and allowed surface preservation. Heavily doped silicon tips (910M-ACTA) with aluminum coating 30 nm thick (force constant 40 N/m, resonance frequency 300 kHz) were used. The tip radius of curvature reported by the manufacturer is less than 10 nm. Images were recorded at a scan rate of 0.3 Hz and a resolution of 256 x 256 pixels. For a 3 x 3 micron scan area, one pixel in a 256 x 256 image corresponds to an area of 11.7 nm x 11.7 nm. XEI program was used for image processing and measurements of the acquired data.

B- Particle size analysis

Particle size analysis of re-dispersed NPsSiO₂ was investigated with a Brookhaven 90Plus Particle Size Analyzer, based on the principles of Dynamic Light Scattering (DLS) Hydrodynamic diameter of SiO₂NPs was 199 \pm 7 nm with 0.005 polydispersity index (PDI).



Fig. S2. Size distribution of SiO₂ nanoparticles at pH=9 in aqueous suspension as obtained from the DLS analysis

C- SEM images





Fig. S3. SEM micrographs of silica nanoparticles

Fig. S4. Proposed sintering mechanism of two SiO₂ nanoparticles



Figure S5. (A) original 2D SEM micrograph, (B) Illustrator processed image, (C) Illustrator processed image and (D) threshold image after eliminating noise using ImageJ

D- AFM images

The following AFM image shows the height profile of the line drawn on the micrograph. As can be seen, the height measured in the center of each nanoparticle coincides with the fact of having a monolayer, with a height value of 200 nm that matches the nominal dimensions of the deposited nanoparticles.



Fig. S6. AFM image of the sample Au_SiO_2 and line profile.

A higher resolution image shows the non-porous structure of the nanoparticles, at least above the resolution that can be achieved with the dimensions of the tip used.



Fig S7. AFM image of the sample Au_SiO_2

E- Theoretical studies



Fig. S8. Theoretical IR spectrum of a SiO₂@CO₂ fragment

F- XPS analysis

Table S1. Electron Binding Energy (eV) and atomic/group percentages for each step of the process

	Au_linker		Au_SiO ₂		Au_SiO ₂ @CO ₂		Assignment
	BE (eV)	%	BE (eV)	%	BE (eV)	%	Acorginiton
	284.3	69	284.4	65.5	284.4	67.8	C-C
C 1s	286.3	23	286.5	29.0	286.4	21.2	C-O-C
	288.6	8	288.7	5.4	288.5	11.0	C=O