

Erratum: Correlating the Morphological Evolution of Individual Catalyst Particles to the Kinetic Behavior of Metallocene-Based Ethylene Polymerization Catalysts (JACS Au (2021) 1:

Original

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Correction to “Correlating the Morphological Evolution of Individual Catalyst Particles to the Kinetic Behavior of Metallocene-Based Ethylene Polymerization Catalysts”

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Supporting Information

Figure 1 in the original paper shows *d*-acetonitrile molecules with four bonds between the N and C atoms. This has been corrected here.

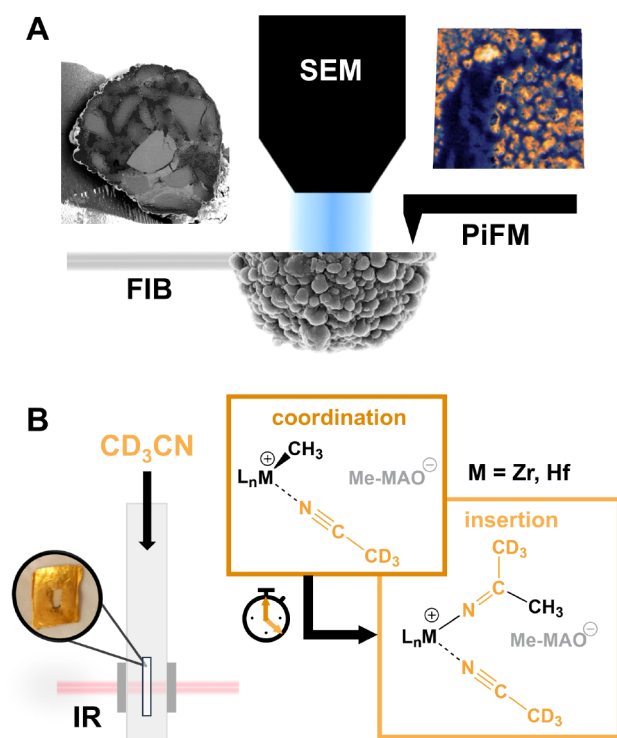


Figure 1. Schematic overview of the multiscale characterization approach applied to the $SiO_2/MAO/M$ ($M = Hf, Zr$) ethylene polymerization catalysts and the information provided by each technique. (A) Correlated focused ion beam–scanning electron microscopy (FIB–SEM) and infrared photoinduced force microscopy (IR PiFM). (B) Time-resolved IR spectroscopy in the presence of *d*-acetonitrile (*d*-ACN) as a probe molecule.

Figure 5 in the original paper featured averaged and smoothed point spectra that were recorded at various different locations on the sample. The figure has been replaced with a

new figure to demonstrate a direct correlation between the point spectra and IR maps that were recorded on the given particle cross-section. The main text was adapted as follows: “Point spectra, recorded of PE- (i.e., A1 and B1 in Figure 5) and silica-rich regions (i.e., A2 and B2 in Figure 5) as well as reference materials (Figures S10–S12), further helped to assign the imaged phases.”

A correction to the Supporting Information, section S4.B, was made to reflect that all data were recorded in PiF and not PiFM mode:

“Atomic force microscopy (AFM) topography images, IR maps and IR point spectra were recorded in dynamic noncontact PiF mode (60 accumulations, 500 ms pixel dwell time, 1 cm^{-1} spectral resolution) using NCHR Au-coated cantilevers (force constant: $\sim 40\text{ N/m}$).”

The “PiFM” labels in Figures S7–S9 (Supporting Information) were changed to “PiF”. Furthermore, the methodology for recording an IR map at a specific wavenumber was described in more detail, both in the Supporting Information and in the main text:

“Prior to acquiring an IR map at a specific wavenumber, a preliminary low-resolution scan was performed. A point spectrum was then taken in the mapped area to determine the wavenumber of the targeted vibrational band (i.e., the wavenumber at which the band has its maximum intensity).”

“The IR PiFM maps were recorded in noncontact mode²⁶ (amplitude ratio set point of 80%, attractive van der Waals force regime; Table S3) at characteristic wavenumbers for the Si–O stretching vibration^{46,47} (maps recorded at single wavenumbers in the range of $1050\text{--}1030\text{ cm}^{-1}$, $\nu(\text{Si–O})$, Figure 4A’–C’) and the symmetric C–H bending vibration of the methylene group^{37–39} (maps recorded at single wavenumbers in the range of $1472\text{--}1460\text{ cm}^{-1}$, $\delta(\text{C–H})$, Figure 4A’’–C’’).”

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“Figure 4. Local catalyst morphology as recorded by scanning electron microscopy (SEM; A, B, C), chemical composition as imaged by infrared photoinduced force microscopy (IR PiFM) [$\nu(\text{Si-O})$]: IR maps recorded at single wavenumbers in the range of 1050–1030 cm^{-1} , A'–C'); $\delta(\text{C-H})$, IR maps recorded at single wavenumbers in the range of 1472–1460 cm^{-1} , A''–C''] and relative mechanical properties as determined by phase shift imaging (A'''–C''').”

In Figures S10–S12 of the Supporting Information, the X-axis label was changed from wavelength to wavenumber.

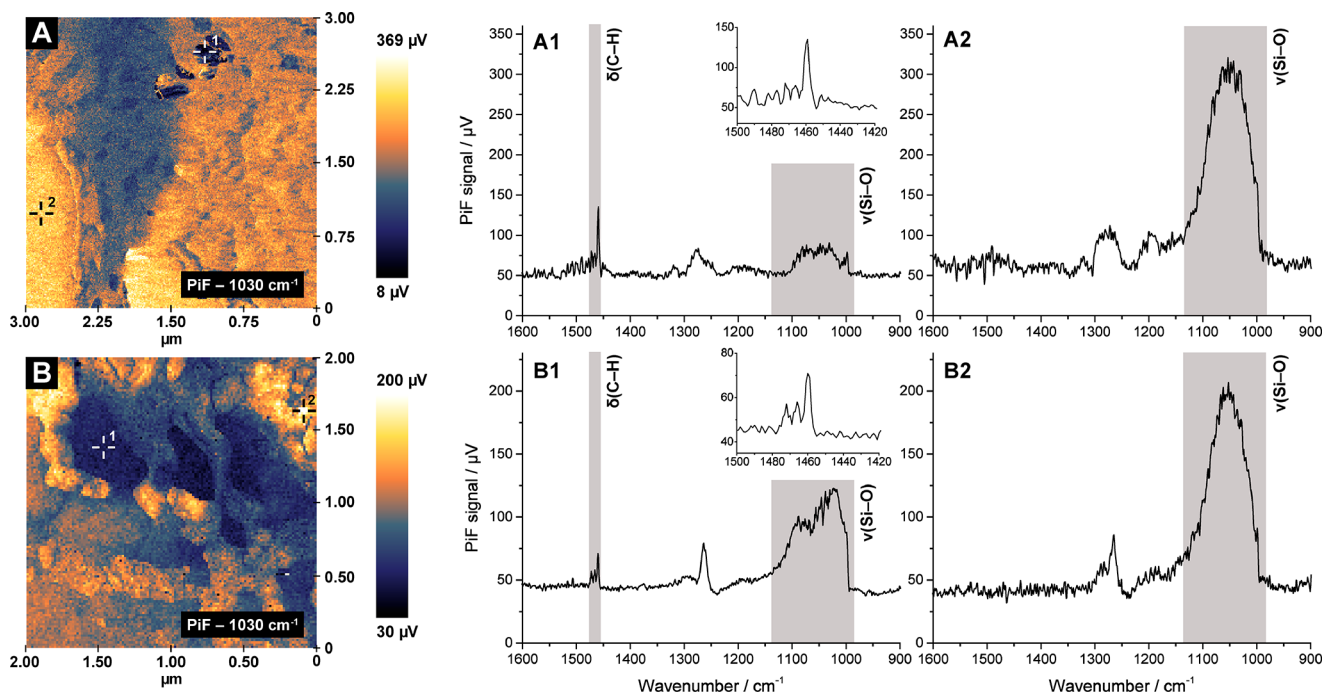


Figure 5. Infrared photoinduced force microscopy (IR PiFM) maps of two different areas of the 30 min prepolymerized hafnocene-based catalyst particle cross-section recorded at 1030 cm^{-1} [$\nu(\text{Si-O})$]. Point spectra (A1, A2, B1 and B2) that were taken at the locations indicated in the IR maps feature vibrational bands of polyethylene (PE) and silica (SiO_2). A second-order Savitzky–Golay filter (5 points) was applied to decrease the level of background noise in the acquired spectra.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/jacsau.3c00266>.

Corrected Figures S10–S12 (PDF)