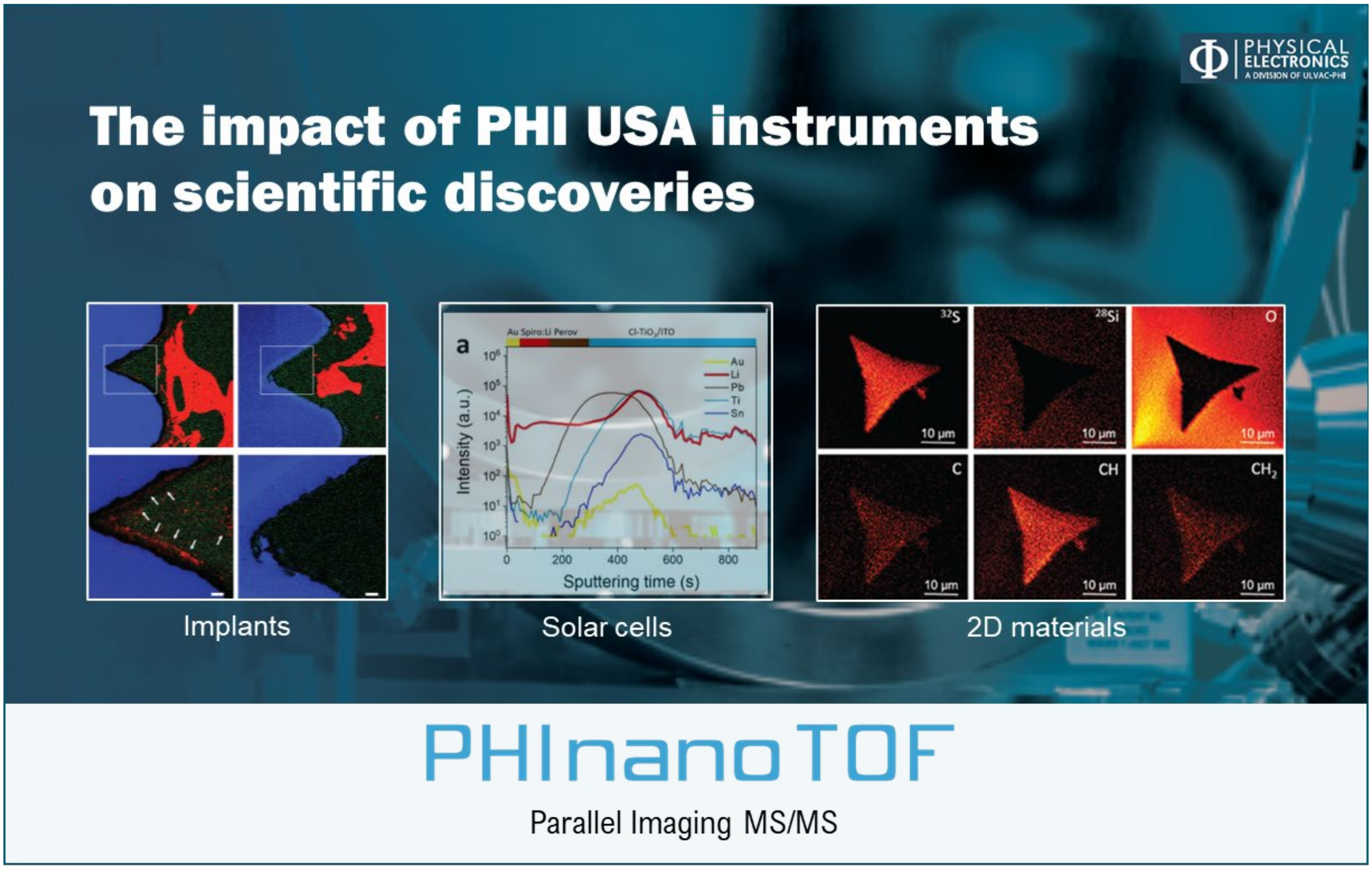

The impact of PHI USA instruments on scientific discoveries

Implants

Solar cells

2D materials

PHI nanoTOF

Parallel Imaging MS/MS

We are looking back at the impact of Physical Electronics TOF-SIMS instruments in supporting scientific publications in the year 2021. Over 900 scholar publications, including peer-reviewed articles and book chapters, have been published in 2021 using PHI *nanoTOF* instruments. PHI TOF-SIMS instruments were used to study a large range of materials for applications of high technological and research importance - solar cells based on perovskites[1-3], 2D materials[4], biological materials[5,6], and batteries.[7-9] Here we would like to highlight a few papers that demonstrate the unique capabilities of PHI *nanoTOF* instruments.

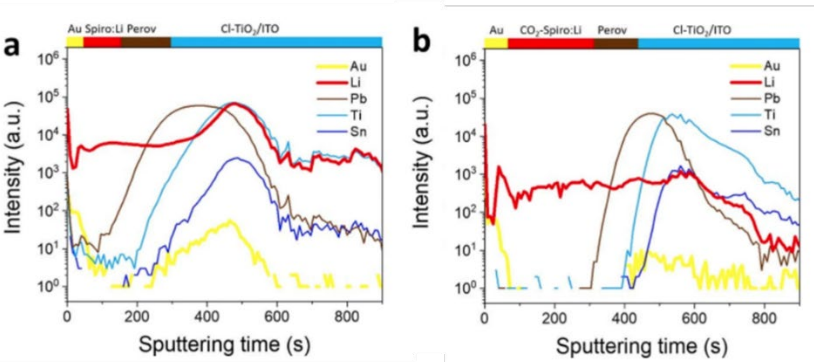

Figure 1. *TOF-SIMS depth profile of pristine solar cell (a) and CO2-treated layer (b).*

In the first paper published in Nature (cited 6 times in the first year), our customers from New York University Tandon School of Engineering used a PHI *nanoTOF* II instrument as well as a PHI *VersaProbe* to study perovskite based solar cells[1]. They conducted TOF-SIMS depth profiling to demonstrate how reducing the content of lithium ions in the hole-transporting layers (HTL) lowered the overall content in the vertical device direction. "*Lithium ions intercalating into the perovskite active layer can result in decomposition of the perovskite and formation of metallic lead, creating recombination sites. The lithium ions were concentrated in particular in the bottom contact layers* (Figure 1a), *which has been shown to result in device failure*." Authors demonstrated that carbon dioxide doping results in a device in which lithium-ion signal is much lower with a minimum accumulation of lithium ions in the bottom contact layers (Fig. 1b).

Another paper published in Advanced Electronic Materials is focused on functionalization of 2D materials, such as MoS_2 and WSe_2.[4] Authors from the University of Bundeswehr combined atomic force microscopy-infrared (AFM-IR) spectroscopy and monolayer sensitive TOF-SIMS, to "*overcome the limitations of classical surface analysis and prove the hi* *ghly selective functionalization of the 2D material surface, which is preferred over the substrate.*" In Figure 2, the elemental maps of negative secondary ions $^{32}S^-$, $^{28}Si^-$, O^-, C^-, CH^-, and CH_2^- were collected from a single, clearly distinguishable, PBI functionalized, and CVD-grown MoS_2 flake on a SiO_2/Si substrate. This paper highlighted the great potential of unconventional techniques such as TOF-SIMS in the field of 2D materials and organic SAMs.

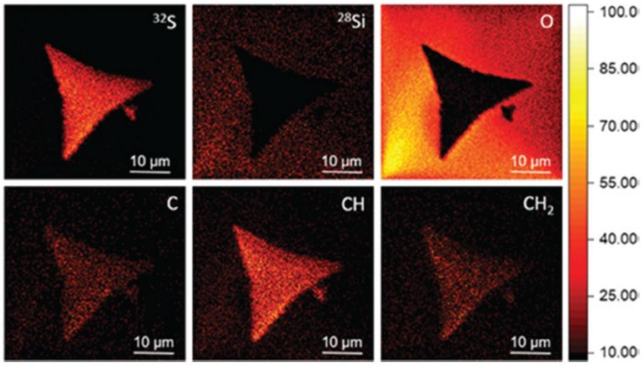

Figure 2. *High resolution TOF-SIMS maps of $^{32}S^-$, $^{28}Si^-$, O^-, C^-, CH^-, and CH_2^- secondary ions*

The third paper we would like to highlight is published by authors from Small Engineering & Sejong Battery Institute and focuses on improving stability of Ni-rich cathodes for lithium-ion batteries. The authors used hydroxyapatite as a coating material, which showed excellent chemical and mechanical properties that provide a suitable coating medium for Ni-rich cathode materials. $LiOH^+$ (m/z = 24.01), $LiOH_2^+$ (m/z = 25.01), and $LiCO_2^+$(m/z = 51.00) fragments, corresponding to the residual lithium compounds, emerged to be significantly high for the bare material relative to the coated materials (Figure 3d). Fragments from lithium-doped hydroxyapatite were also detected (Figure 3e). These fragments were not observed for the uncoated cathode. In addition, TOF-SIMS was used to study the surface of the coating after electrochemical reaction for 500 and 1000 cycles. The formation of fluorinated $Ca_{4.67}Li_{0.33}(PO_4)_3F$ and CaF_2 layers was found to be related to morphological stability.

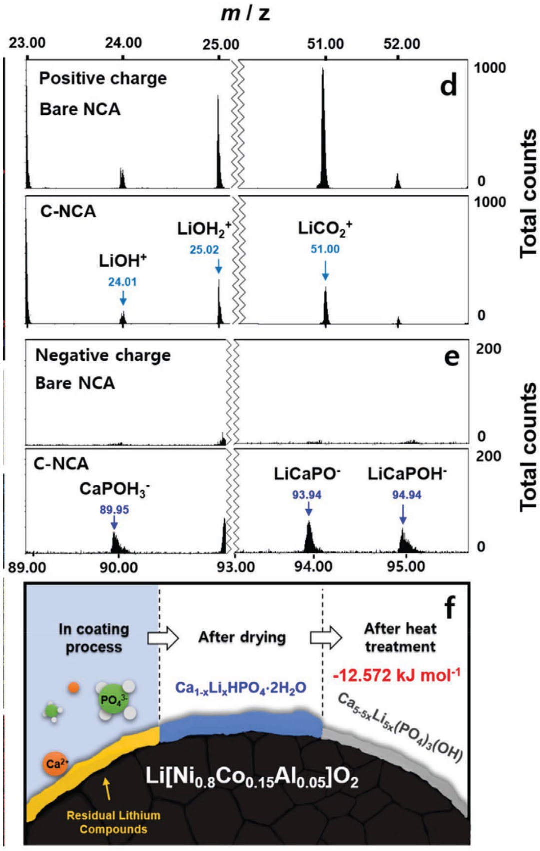

Figure 3. *ToF-SIMS results of bare and hydroxyapatite coated cathode powders, (d) positive fragments: $LiOH^+$, $LiOH_2^+$, $LiCO_2^+$, (e) negative fragments: $CaPOH_3^-$, $LiCaPO^-$, $LiCaPOH^-$ fragments (top: bare; bottom: coated) (f) Schematic illustration for the detailed modification process.*

Read more about these and other discoveries in the papers cited below.

1. https://www.nature.com/articles/s41586-021-03518-y#Sec26
2. https://onlinelibrary.wiley.com/doi/abs/10.1002/aenm.202101454
3. https://doi.org/10.1038/s41566-021-00857-0
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