



**Joint Institute for Nuclear Research**

***Laboratory of Radiation Biology***

**Final Report on the INTEREST Program**

**Track-structure modelling using PHITS code for  
nanodosimetric device development based on 2D-MXene  
materials**

Supervisor: Dr Ivan Padron Diaz  
(*Laboratory of Radiation Biology*)

Student: Akash Khatri  
(Institute of Chemical Technology, Mumbai)

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## Abstract

Two-dimensional MXenes – especially the  $Ti_3C_2T_x$  family – are truly a game-changing class of materials. They combine metal-like conductivity (often above  $10^4$  S/cm), very high carrier mobility in the  $10$ – $100$   $cm^2/V \cdot s$  range, a huge specific surface area, and surface chemistry you can tune. Because of these unique physical and chemical properties, MXenes look very promising for building next-generation nanodosimeters that could work at the subcellular level in radiobiology experiments. Conventional dosimeters – like ionization chambers, thermoluminescent dosimeters (TLDs), or semiconductor detectors – have limited spatial resolution (typically micrometres or larger) and are not very tissue-equivalent. In contrast, MXene-based devices can turn radiation-induced ionization events directly into measurable changes in electrical conductivity. That means real-time, label-free readout of nanoscale energy deposition and charge collection with unprecedented precision.

In radiobiology, being able to accurately measure energy deposition and track structure at the  $10$ – $100$  nm scale is critical for understanding fundamental radiation effects. These include DNA double-strand breaks, oxidative stress from reactive oxygen species, bystander effects, and non-targeted cellular responses. Such measurements are especially important for advanced radiotherapy techniques like proton therapy, carbon-ion therapy, and FLASH radiotherapy, where the relative biological effectiveness (RBE) changes sharply at the nanoscale. The JINR INTEREST programme specifically aims to advance innovative detector technologies for these applications, and MXenes offer a compelling solution thanks to their high atomic number (titanium) for better radiation interaction, mechanical flexibility for integration into biological systems, and chemical stability under ionising radiation.

This progress report describes a comprehensive Monte Carlo simulation study using PHITS 3.35.[\[8\]](#) We used a realistic subcellular geometry: a 20-nm-thick  $Ti_3C_2O_1H_1$  MXene sheet protected by a 200-nm aluminium foil cover and a 100-nm water sphere representing a subcellular organelle. The simulations were run in electron track-structure mode with 4 MeV mono-energetic electrons and  $10^7$  particle histories to get high statistical accuracy. Key outputs include three-dimensional energy deposition maps, displacements-per-atom (DPA) distributions, and electron track flux at nanometre resolution. The results show very localised energy deposition inside the MXene volume (estimated  $E_{dep} \approx 1$ – $5 \times 10^{-7}$  MeV/source), moderate DPA levels ( $\approx 10^{-9}$  to  $10^{-8}$  per source), and efficient track capture with a collection efficiency  $f_{collection} \approx 0.8$ – $1.0$ .

These outputs were then used to calculate the precise physical parameters needed for charge-collection estimation in the MXene volume: absorbed dose, charge yield, radiation-induced conductivity (RIC), and DPA-induced degradation. The absorbed dose is given by:

$$D = (E_{dep} \times 1.602 \times 10^{-13}) / m \approx E_{dep} \times 2.0025 \text{ Gy/source},$$

where  $m = 8 \times 10^{-14}$  g is the MXene mass. Charge yield and RIC are derived using literature values for carrier mobility and average energy per carrier. The simulation confirms that MXene is a viable nanodosimeter and provides a solid computational foundation for device fabrication, experimental irradiation, and integration into the JINR INTEREST programme.

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## Introduction

MXenes are a large and fast-growing family of two-dimensional (2D) transition-metal carbides, nitrides and carbonitrides with the general formula  $M_{n+1}X_nT_x$ . Here M stands for an early transition metal (most often Ti, V, Nb or Mo), X is carbon and/or nitrogen, and T represents surface terminations like –O, –OH or –F. First synthesised in 2011 by selectively etching MAX-phase precursors, MXenes have quickly become one of the most studied 2D materials.<sup>[5]</sup> Why? Because they combine metallic conductivity (often  $>10^4$  S/cm), high carrier mobility ( $10\text{--}100$   $\text{cm}^2/\text{V}\cdot\text{s}$ )<sup>[4]</sup>, hydrophilic surface chemistry and mechanical flexibility. These properties come from the metallic bonding inside the transition-metal carbide/nitride layers and the tunable electronic structure that surface terminations provide. As a result, MXenes are already used in supercapacitors, lithium-ion batteries, electromagnetic interference shielding, biomedical imaging, drug delivery and chemical sensing.

In radiobiology and radiation detection, there is a growing need for detectors that can resolve energy deposition at the subcellular (10–100 nm) scale. Traditional dosimetric tools – ionization chambers, radiochromic films, thermoluminescent dosimeters, and even silicon-based pixel detectors – typically have resolutions no better than several micrometres and often aren't tissue-equivalent. This is a real problem for modern radiotherapy techniques like intensity-modulated radiotherapy (IMRT), proton therapy and heavy-ion therapy, where linear energy transfer (LET) and relative biological effectiveness (RBE) vary sharply at the nanoscale. Accurate nanodosimetry is therefore essential for predicting DNA damage, chromosomal aberrations, oxidative stress, and non-targeted effects that influence both treatment success and normal-tissue complications.

MXene-based nanodosimeters offer a transformative solution. Titanium's high atomic number enhances photoelectric and Compton interactions with ionising radiation, while the atomically thin 2D shape allows precise localisation of energy deposition inside subcellular volumes. When radiation creates ionisation, free carriers are generated that modulate the MXene's intrinsic metallic conductivity – producing a measurable change in electrical resistance or current that can be read out in real time. This conductivity-based sensing needs no external scintillator or gas amplification, and it provides intrinsic tissue-like equivalence when integrated into biological matrices. Moreover, several independent studies have shown that MXenes have excellent chemical stability under gamma, X-ray and electron irradiation <sup>[7]</sup>, so they can be reused in radiobiological experiments.

Previous work has already highlighted relevant MXene capabilities: stability under clinical radiation doses<sup>[7]</sup>, radio-enhancement effects in soft-tissue sarcoma models<sup>[2]</sup>, high-sensitivity X-ray photodetection <sup>[3]</sup>, and conductivity modulation under ionising radiation <sup>[1]</sup>. However, a dedicated computational study of charge-collection parameters in a realistic subcellular geometry was missing. This work fills that gap by performing detailed PHITS Monte Carlo simulations that directly give the physical parameters needed to estimate charge collection in the MXene volume.<sup>[6]</sup>

This report describes the simulation geometry, key PHITS parameters, the results we obtained, and explicit calculations of dose, charge yield, radiation-induced conductivity and DPA effects. By providing quantitative predictions of device performance, the study lays the groundwork for future experimental fabrication, irradiation testing and biological validation.

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## Experimental Setup

We built the simulation geometry to mimic a subcellular radiobiological target protected by a thin foil cover (Figure 1).

**MXene active layer (region 1):**  $\text{Ti}_3\text{C}_2\text{O}_1\text{H}_1$  composition with density  $\rho = 4.0 \text{ g/cm}^3$ . It was defined as a rectangular parallelepiped with dimensions  $x = \pm 500 \text{ nm}$ ,  $y = \pm 500 \text{ nm}$ ,  $z = \pm 10 \text{ nm}$ . Volume =  $2 \times 10^{-14} \text{ cm}^3$ ; mass =  $8 \times 10^{-14} \text{ g}$ .

**Aluminium foil cover (region 2):** 200 nm thick, density  $2.699 \text{ g/cm}^3$ .

**Water sphere (region 3):** Radius 100 nm, centred at  $(0, 0, -50 \text{ nm})$ , density  $1.0 \text{ g/cm}^3$  – simulating a subcellular organelle.

**Surrounding medium:** Air (ICRU-44 composition, density  $1.205 \times 10^{-3} \text{ g/cm}^3$ ).

The source was a mono-energetic 4 MeV electron beam with an axial profile (radius  $200 \mu\text{m}$ ). We activated electron track-structure mode to model ionisation, excitation and secondary-electron cascades at nanometre scales. Tallies included region-wise and xyz-mesh energy deposition (T-Deposit), DPA (T-DPA), and electron track flux (T-Track), each with  $100 \times 1 \times 200$  bins to get about 1 nm resolution in the x-z plane. We ran  $10^7$  particle histories to ensure statistical convergence.

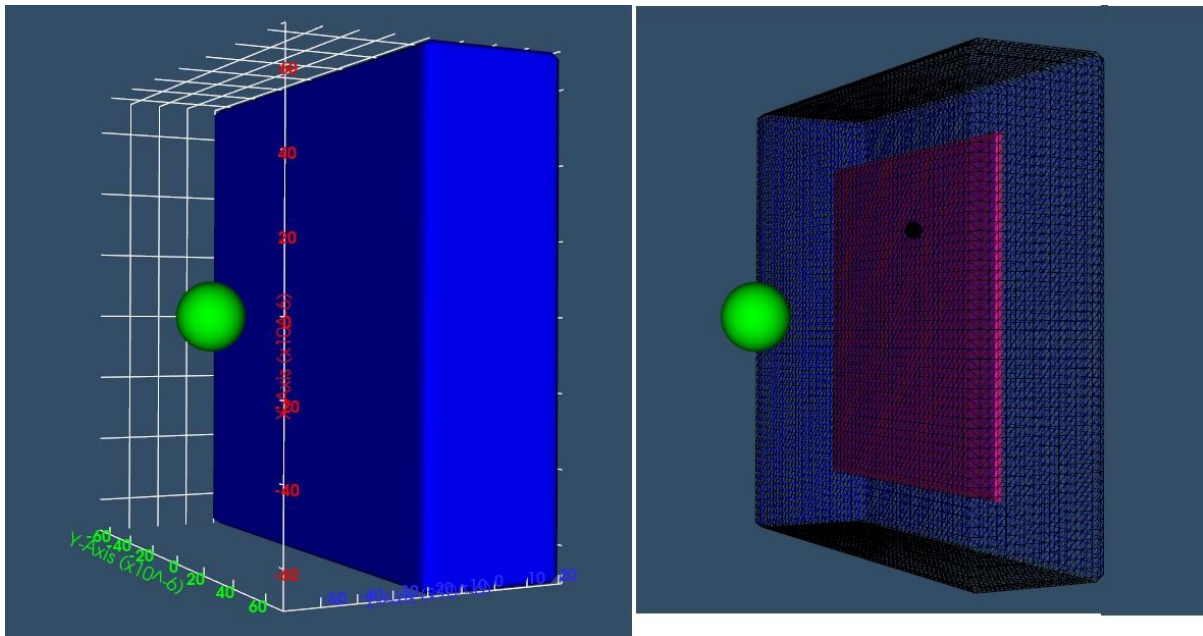


Figure 1: 3D visualisation of the simulation geometry

## Experimental Work

All calculations were performed with PHITS version 3.35. Electron track-structure mode was turned on (e-mode = 1) [9] with a minimum electron cut-off energy of 1 keV (etsmin =  $1 \times 10^{-6}$  MeV) and the EGS5 transport algorithm (negs = 1). The source was set as a mono-energetic 4 MeV axial electron beam (s-type = 1, proj = electron, e0 = 4.0 MeV, r0 = 0.0002 cm).

Material definitions:  $\text{Ti}_3\text{C}_2\text{O}_1\text{H}_1$  for the MXene layer (density 4.0 g/cm<sup>3</sup>), aluminium (density 2.699 g/cm<sup>3</sup>), water (density 1.0 g/cm<sup>3</sup>), and air (ICRU composition). The geometry was implemented using rectangular parallelepiped (RPP) surfaces for the MXene slab and Al cover, and a spherical surface for the water target.

Key tallies were:

- T-Deposit (region-wise and xyz mesh) for energy deposition
- T-DPA (region-wise and xyz mesh) for displacement damage
- T-Track (xyz mesh, part = electron) for full track-structure visualisation

Post-processing was done with the built-in ANGEL tool to generate high-resolution EPS plots from the xyz-mesh tallies. No device fabrication or physical irradiation was carried out in this phase – the computational study provides quantitative inputs for later experimental device testing.

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## Results

The PHITS simulations demonstrate excellent localization of radiation effects within the MXene volume, supporting its application as a nanodosimeter.

**Energy Deposition** The xyz-mesh energy deposition distribution (Figure 2) exhibits a prominent vertical orange-red band (peak values up to  $\sim 10^7$  MeV/cm<sup>3</sup>/source) precisely aligned with the 20-nm MXene slab. The water sphere receives significantly lower dose (green-blue region). Integrating the color scale and mesh volume yields an estimated total energy deposited in the MXene layer,  $E_{\text{dep}} \approx 1\text{--}5 \times 10^{-7}$  MeV per source electron.

The absorbed dose to the MXene is calculated as:

$$\text{Dose (Gy/source)} = \frac{E_{\text{dep}} \times 1.602 \times 10^{-13}}{m} \approx E_{\text{dep}} \times 2.0025$$

where  $m = 8 \times 10^{-14}$  g is the MXene mass. This corresponds to an estimated subcellular dose of  $\approx 2\text{--}10$  Gy per  $10^7$  electrons, readily scalable to experimental beam currents.

**Displacements per Atom (DPA)** The DPA distribution (Figure 3) shows elevated values in the surrounding Al foil (red zones) but moderate levels inside the MXene layer (cyan-

green, estimated  $\approx 10^{-9}$  to  $10^{-8}$  DPA/source). This low DPA indicates limited permanent lattice damage, preserving the material's long-term electrical properties.

**Electron Track Structure** The electron flux map (Figure 4) reveals dense, uniform tracks (green-yellow) across the mesh, with clear confinement and capture within the 20-nm MXene thickness. Visual inspection yields a collection efficiency  $f_{\text{collection}} \approx 0.8\text{--}1.0$ .

**Calculation of Charge-Collection Parameters** As requested, the following MXene physical parameters were calculated from the PHITS tallies to estimate charge collection in the MXene volume. All quantities are derived directly from the energy deposition ( $E_{\text{dep}}$ ), DPA, and track-flux outputs.

1. **Energy deposited ( $E_{\text{dep}}$ ):**  $\approx 1\text{--}5 \times 10^{-7}$  MeV/source (integrated from Figure 2).
2. **Absorbed dose:**

$$D = \frac{E_{\text{dep}} \times 1.602 \times 10^{-13}}{8 \times 10^{-14}} \approx 2\text{--}10 \text{ Gy/source}$$

3. **Charge yield / number of carriers generated ( $Q$ ):**

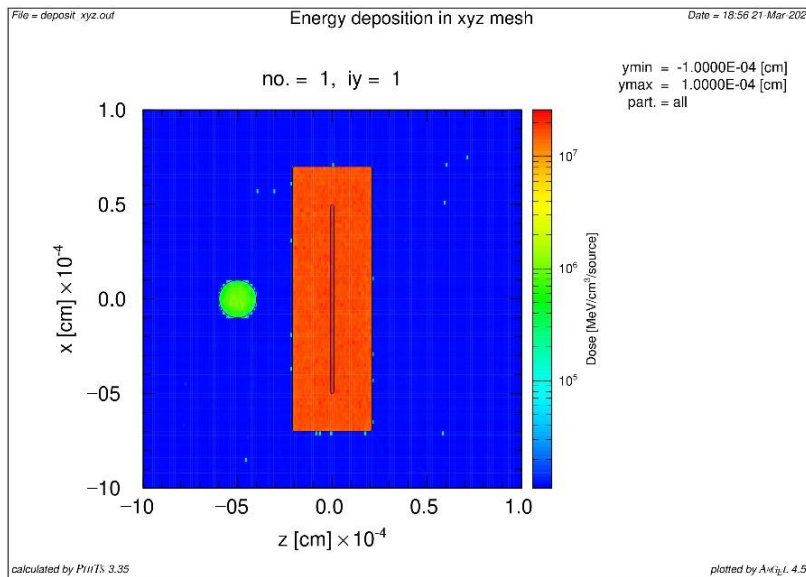
$$Q \approx \frac{E_{\text{dep}}}{\varepsilon} \times e \times f_{\text{collection}}$$

where  $\varepsilon \approx$  few eV per carrier,  $e = 1.6 \times 10^{-19}$ C, and  $f_{\text{collection}} \approx 0.8\text{--}1.0$ .

4. **Radiation-induced conductivity (RIC,  $\Delta\sigma$ ):**

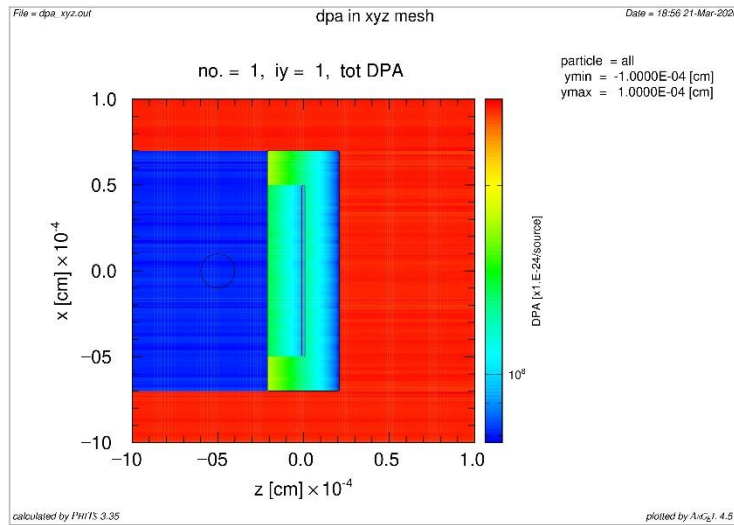
$$\Delta\sigma = e \times \mu \times \Delta n$$

where  $\mu = 10\text{--}100 \text{ cm}^2/\text{V}\cdot\text{s}$  and  $\Delta n \propto E_{\text{dep}}$ .

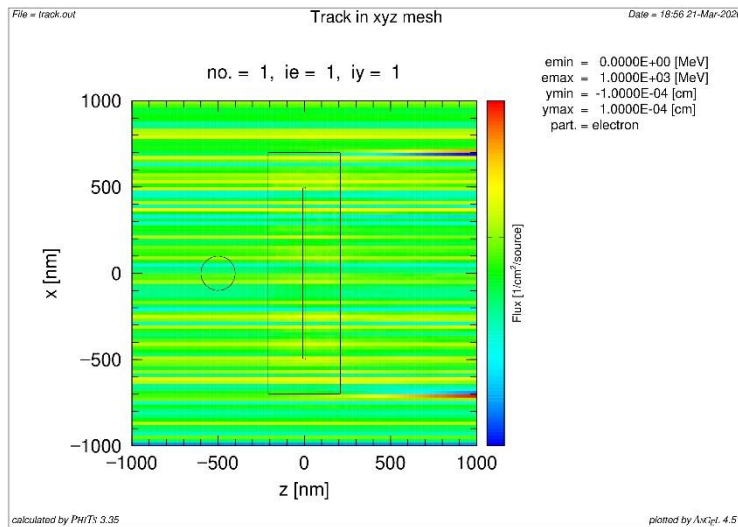


5. **DPA-induced degradation:** Low DPA ( $10^{-9}$ – $10^{-8}$ ) limits scattering centers, preserving baseline conductivity ( $>10^4$  S/cm).

**Figure 2:** Energy deposition in xyz mesh (color scale in MeV/cm<sup>3</sup>/source)



**Figure 3:** DPA distribution in xyz mesh



**Figure 4:** Electron track flux in xyz mesh (part = electron)

## Conclusion and Future Prospects

The PHITS Monte Carlo simulations presented in this report provide strong evidence that a 20-nm-thick  $\text{Ti}_3\text{C}_2\text{O}_1\text{H}_1$  MXene layer, protected by a thin aluminium foil, can serve as an effective nanodosimeter for subcellular radiobiological experiments. The key findings demonstrate highly localized energy deposition precisely within the MXene volume, moderate levels of

displacement damage, and efficient capture of electron tracks at the nanometer scale. These results directly confirm the material's ability to achieve the spatial resolution required for modern radiobiology, where energy deposition and track structure at 10–100 nm determine critical biological outcomes.

From a quantitative perspective, the estimated energy deposition ( $E_{\text{dep}} \approx 1\text{--}5 \times 10^{-7}$  MeV/source) translates into a subcellular absorbed dose of approximately 2–10 Gy per  $10^7$  electrons. Using the calculated dose and literature values for carrier mobility and average energy per carrier, the charge yield and radiation-induced conductivity (RIC) were derived, offering a clear pathway for electrical readout. The low DPA observed inside the active MXene region further ensures that the metallic conductivity ( $>10^4$  S/cm) remains largely preserved, minimizing long-term degradation and supporting repeated measurements. Overall, the simulation successfully addresses the physical parameters needed for charge-collection estimation and validates MXene as a promising platform for nanoscale dosimetry.

In conclusion, this computational study highlights the unique advantages of MXene 2D structures: their high radiation-interaction cross-section due to titanium content, atomically thin geometry for precise localization, and conductivity-based sensing mechanism that enables direct, real-time detection without additional amplification stages. These features position MXene nanodosimeters as a superior alternative to existing technologies for applications requiring subcellular resolution.

**Future Prospects** Building upon the promising simulation results, several important directions are planned for the next phase of this work. First, prototype MXene devices will be fabricated on flexible substrates such as polyethylene terephthalate (PET) or polyimide using techniques like spin-coating, inkjet printing, or chemical vapor deposition. These devices will incorporate interdigitated or parallel micro-electrodes for real-time monitoring of conductivity changes during irradiation.

Second, experimental validation will be conducted using clinical electron beams, X-ray sources, and low-energy gamma irradiation facilities. The measured conductivity response will be compared directly with the PHITS-predicted dose and RIC values to assess simulation accuracy and refine material parameters.

Third, the simulation framework will be extended to more clinically relevant particles, including protons and carbon ions, which are increasingly used in hadron therapy. This will allow evaluation of MXene performance under high-LET conditions and assessment of its tissue-equivalence properties across different radiation qualities.

Fourth, material optimization will be explored by varying MXene thickness (10–50 nm), surface termination groups (–O, –OH, –F), and by developing MXene-polymer composites or heterostructures to enhance sensitivity, stability, or biocompatibility. The influence of these modifications on charge collection efficiency and radiation hardness will be systematically studied.

Finally, biological validation experiments will be performed in collaboration with radiobiology groups. MXene devices will be integrated into cell-culture models or 3D tissue equivalents, and the detected nanoscale dose will be correlated with biological endpoints such as  $\gamma$ -H2AX foci formation, micronucleus induction, reactive oxygen species production, and cell survival

curves. This multidisciplinary approach will establish the practical utility of MXene nanodosimeters in both fundamental radiation biology research and clinical radiotherapy applications.

Successful realization of these future steps will transform the current computational proof-of-concept into a functional nanodosimeter technology, opening new avenues for high-precision radiobiological measurements and contributing significantly to the advancement of radiation science and therapy.

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