Create a project:
New project→enter polymer_metal oxide→click the OK

Input crystal structure:
Import→Navigate to Structures\metal-oxides→double-click on Al2O3.msi.

Cleave the surface:
Build→Surfaces→Cleave Surface
Cleave plane (h k l)→0 0 -1→change thickness to 13 Å→Cleave and close the dialog (check lattice parameters).

Surface relaxation with Forcite (molecular mechanics)

1. Module→Forcite→Calculation
2. Setup→Task→Geometry Optimization
3. Assigns a forcefield type to each atom: On the Energy tab→Forcefield→select COMPASS→click More to open Forcite Preparation Options dialog→Uncheck "the calculate automatically" (Note: To prevent the bonds between the oxygen and aluminum atoms, which are not parameterized as the structure is ionic.)→click the "Calculate" button→close the dialog.
4. On the Energy tab→make Charges to be assigned by Forcefield.
5. Rotate the model so that the surface is at the top→Select all the atoms apart from the top two rows.
6. Modify→Constraints→Check the Fix Cartesian position→Close the dialog→deselect the atoms.
7. Hold down the ALT key→double-click on any bond→Press the DELETE key to remove the bonds between the aluminum and oxygen atoms.

Relax the surface: Module→Forcite→Calculation→Run.

Increase the surface area and change the periodicity

1. Ensure that the optimized Al2O3 (0 0 -1).xsd→Build | Symmetry | Supercell→ Increase the Supercell range to 3 for both U and V→Create Supercell→Close the dialog.
2. Build→Crystals→Build Vacuum Slab→Change the Vacuum thickness to 0.0→ Build.

Build the polymer:

1. Import→Navigate to Structures\repeat-units\vinyls\styrene.msi→Open.
2. Sketch Fragment→select Fragment Browser→Expand the Functional Groups node→select Nitro dioxide→Click once on the para hydrogen of the phenyl ring→Close the dialog→Rename styrene.xsd to p-nitrostyrene.
3. Use this monomer to build a homopolymer:
   Build | Build Polymers | Homopolymer→Change the Library to Current project, Repeat unit to p-nitrostyrene, Tacticity to Atactic, and the Chain length to 8→Build→Close the dialog.
4. Use Amorphous Cell to obtain realistic polymer conformations:
   Module→Amorphous Cell→select Calculation→Task: choose Confined layer→Composition→Molecule: select the Polyp-nitrostyrene.xsd
   Check the lattice parameters *a* and *b* of the Al2O3(0 0 -1).xsd
   Make Polyp-nitrostyrene.xsd the active document→Click "More" on the Amorphous Cell Calculation dialog→Lattice type Select Orthorhombic→set the values of both *a* and *b* equal to that of the Al2O3(0 0 -1).xsd→On the Setup tab set the Density to 0.8→On the Energy tab set the Forcefield to COMPASS→ Run→Close the dialog.

Add the polymer to the surface:

1. Build | Build Layers to open the Build Layers dialog→set Layer 1: Al2O3 (0 0 -1).xsd; Layer 2: Polyp-nitrostyrene.xtd→On the Layer Details tab, increase the Vacuum for Layer 2 to 30.0→On the Matching tab, select the lattice parameters for Layer 1→Build→Close the Build Layers dialog.
2. Save Project, followed by Window | Close All.

Optimize the layer and run molecular dynamics:

1. Double-click on **Layer.xsd**→Select all the surface atoms→Modify Constraints→uncheck then check the Fix Cartesian position checkbox→Close the dialog and click in the 3D Viewer.
2. Module→Forcite→Calculation→Task: Geometry Optimization→More: set the Max. iterations to 1000→Close the dialog→Run.
3. The generated optimized structure is now ready for the dynamic simulation:
   Module→Forcite→Calculation→Task: Dynamics→More: set the Number of steps to 500→Close the dialog→Run and close the Forcite Calculation dialog. The final structure is present in the **.xtd** document.