DEEPICE – A DEEP NEURAL NETWORK TO INVESTIGATE WATER AND ICE SYSTEMS

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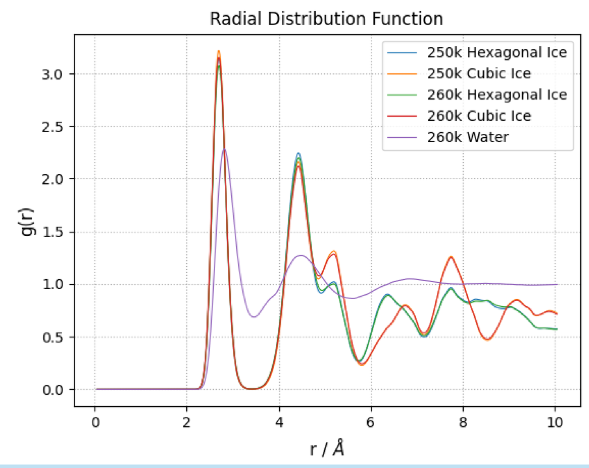
Goal:

To train a **deep neural network** (**DeepIce**) to distinguish **ice**-like and **water**-like molecules in different ice structures, simulated with the **mW potential**. The **thickness** of **quasi-liquid layers (QLLs)** formed on these **surfaces** will be measured for temperatures in the range **200K** to **270K**.

Quasi-liquid layer (QLL) – A layer on the surface of ice, below the melting point, which has solid-like and liquid-like properties. First suggested by Faraday over 160 years ago.

mW Potential – An empirical, course-grain, model of H_2O. It disregards hydrogen atoms & electrostatic interactions. The model is surprisingly accurate with a low computational cost.

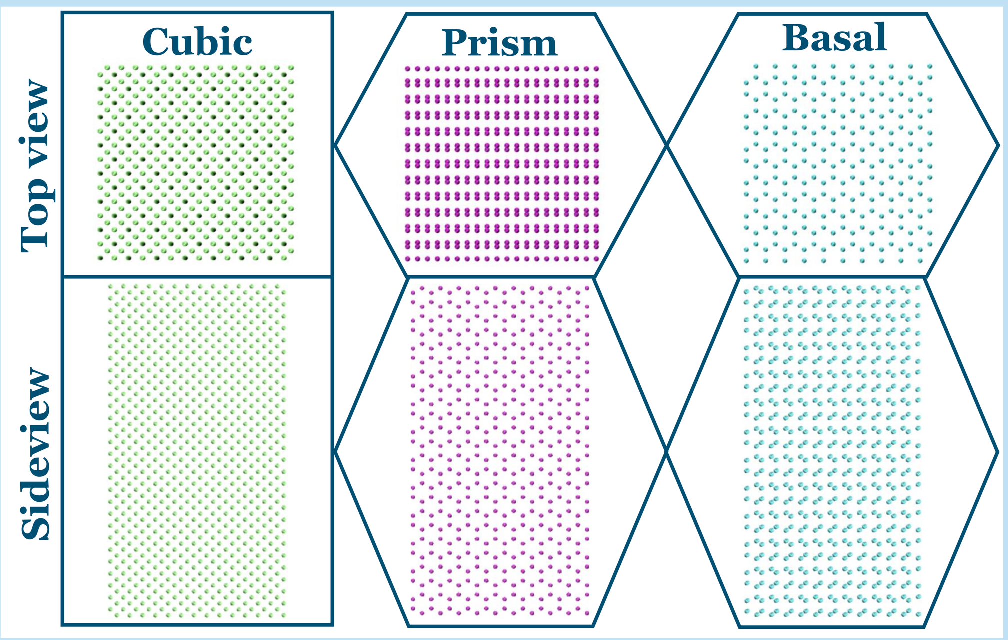
g(r) Radial Pair Distribution – The average number density of molecules at a distance, r, from a reference molecule.



Ice Structures:

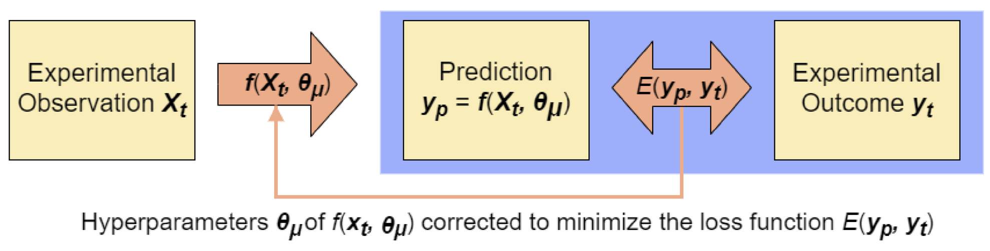
Cubic Ice (Ic)
- Tetrahedral-like structure.
- Meta-stable state of ice.
- Found in the atmosphere of Mars.

Hexagonal Ice (Ih)
- Tetrahedral-like structure.
- Most abundant phase of ice in the Earth's atmosphere.



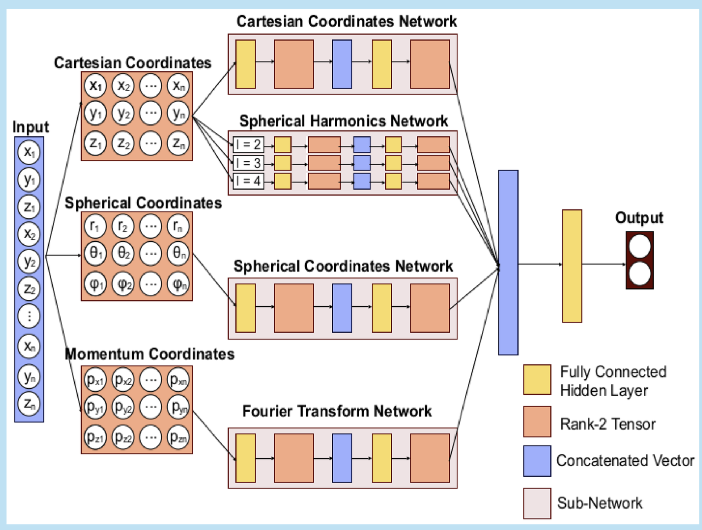
Machine Learning:

Form of data fitting. **Parameters** of a **blackbox** function (**neural network**) are minimized.



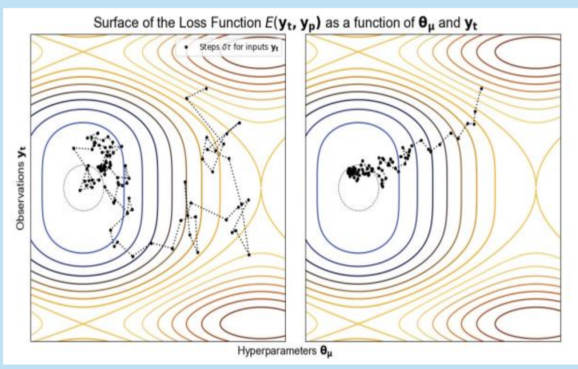
DeepIce:

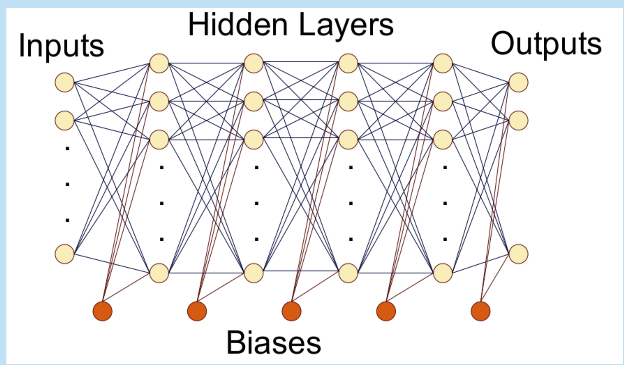
- **DeepIce** is a **deep neural network** scheme composed of **4 sub-networks**.
- It takes as **input** the **coordinates** of the ***n* nearest neighbours** of each **molecule** in the system.
- Each sub-network derives relationships between the molecule's **environment** and its **phase**.
- Classifies each molecule within an **ice-water system**, as **ice-like** or **liquid-like**.



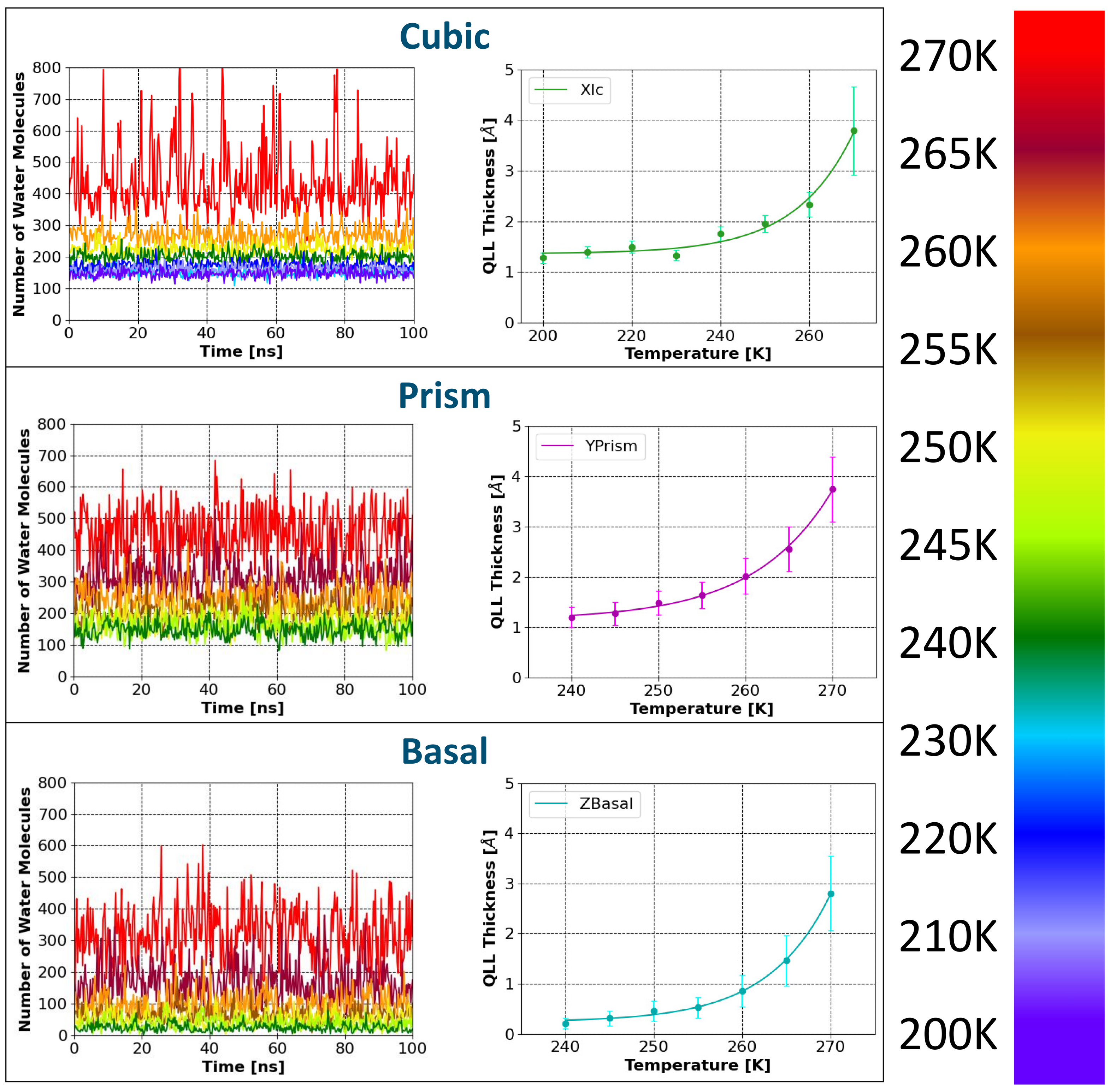
Neural Network:

The number of **degrees of freedom** within the neural network must match the size of the data-set, in order to avoid **mis-fitting**. Achieved by adjusting the number of layers, **neurons**, and **batches**.

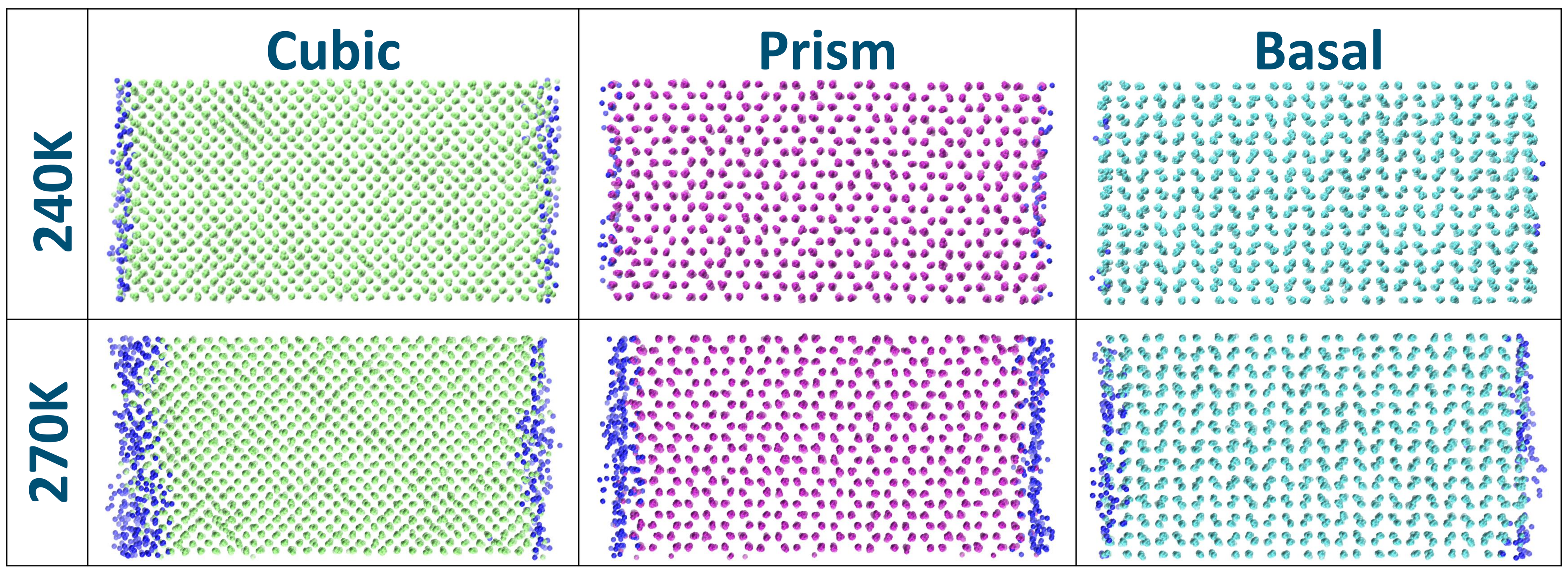




QLL Results:



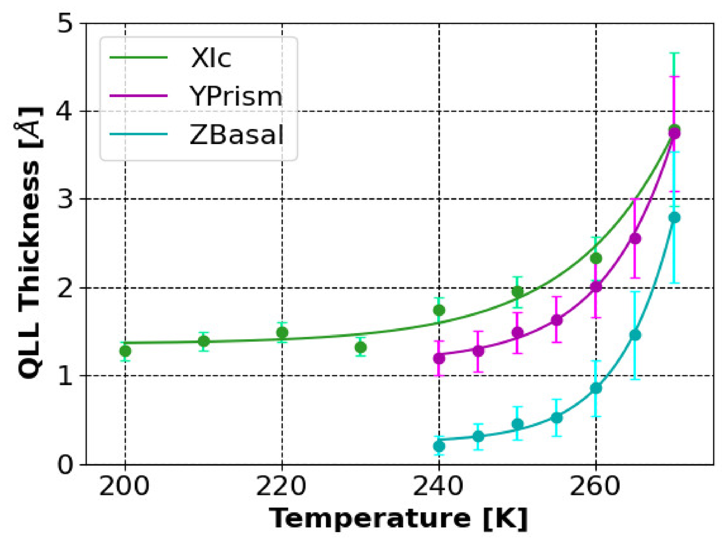
Quasi-Liquid Layer (QLL) Visuals:



Trends on how the number of water molecules and QLL thickness vary are as follows:
- QLL thickness / no. of water molecules increases with temperature.
- QLL thickness / no. of water molecules fluctuates more as temperature increases.
- QLL thickness / no. of water molecules of Cubic > Prism > Basal.

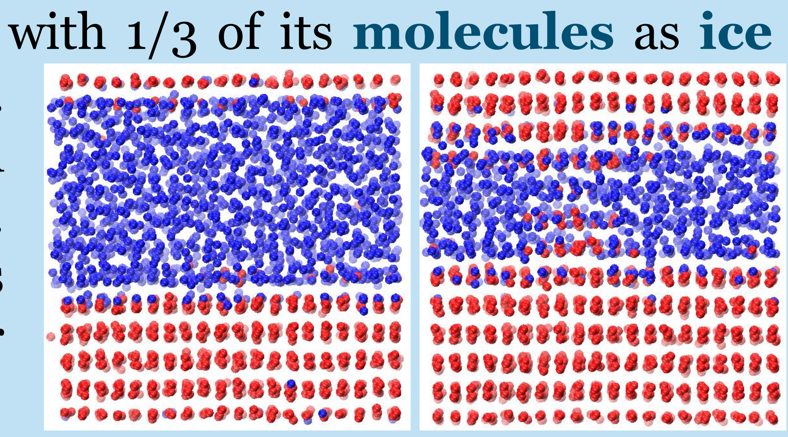
Results:

Our results show that **Cubic Ice** structures have the thickest **QLL** at all **temperatures.** This agrees with experiments that utilised different models of water and molecular **phase** identification.



Crystallisation:

A **slab** with 1/3 of its **molecules** as **ice** (red) and 2/3 as **water** (blue). The slab is held at **260K** and **re-crystallises** over time. **DeepIce** monitors this process by classifying water and ice molecules.



Conclusions and Perspectives:

DeepIce is an insightful **machine learning** algorithm capable of distinguishing between **water** and **ice** molecules on **ice surface slabs,** simulated using the **mW potential**. Using DeepIce, the time-evolution of the number of water molecules on these ice surfaces can be monitored facilitating the calculation of the **QLL thickness** at various temperatures. In the range **200K** to **270K**, the thickness varied between **0.1 Å** and **4.7 Å**.

This project can be furthered by utilising DeepIce to predict upon slabs simulated with the **TIP4P/Ice model**, providing a direct comparison with the mW potential. DeepIce could also be used to visualise how other phase transitions such as **vaporisation**, **sublimation** and **condensation** occur molecule by molecule, as done with crystallisation.

1. Molinero & Moore, Water Modeled As an Intermediate Element between Carbon and Silicon. J. Phys. Chem. B 113(13), 4008–4016 (2009)
2. Fulford et al., DeepIce: A Deep Neural Network Approach To Identify Ice and Water Molecules. J. Chem 59(5), 2141–2149 (2019)
3. Kling et al., Structure and dynamics of the quasi-liquid layer at the surface of ice from molecular simulations. J. Chem. Phys. 122(43), 24780–24787 (2018)