

## Agenda for Site Calculation Meeting

4<sup>th</sup> September, 2020. By Zoom.

Presentations are 20 mins. incl. time for discussion

### Session 1:

<b>9:30:</b>	Opening Remarks	(Leandro Liborio)
<b>9:30 - 9:50:</b>	Leandro Liborio (STFC)	The Ada Lovelace Project on Muon Spectroscopy
<b>9:50 - 10:10:</b>	Alejandra Gonzalez Beltran (STFC)	Requirements for Muon Software
<b>10:10 - 10:30:</b>	Wan Nurfadhilah Zaharim (USM)	Computational Studies on Muonium Trapping Sites in Guanine Base
<b>10:30 - 10:50:</b>	Speaker from Asia (???)	TBC

10:50-11:00 Break

### Session 2:

<b>11:00 - 11:20:</b>	Tom Lancaster (Durham)	Muon Sites in Magnetic Materials: A Summary of Recent Work
<b>11:20 - 11:50:</b>	Ben Huddart (Durham)	MuFinder: A Program to Classify and Analyse Muon Stopping Sites
<b>11:50 - 12:10:</b>	Steve Blundell (Oxford)	Using DFT+mu to study quantum decoherence in non-magnetic fluorides

12:10-13:30 Lunch time + discussions in break-out rooms

### Session 3:

<b>13:30 - 13:50:</b>	Thomas Prokscha (PSI)	Low-energy $\mu$ SR studies at interfaces and the need for DFT calculations for their interpretation
<b>13:50 - 14:10:</b>	Simone Sturniolo (STFC)	Muon stopping sites from symmetry and electrostatics
<b>14:10 - 14:30:</b>	Francis Pratt (STFC)	Computational Software and Computational Results Supporting Muon Spectroscopy

14:30-14:45 Break

Session 4:

**14:45 - 15:05:** Pietro Bonfa (Parma)

**15:05 - 15:25:** Iain McKenzie (TRIUMF)

High-throughput characterization of muon sites

Using DFT calculations and Monte Carlo

simulations to extract information from

ALC- $\mu$ SR spectra about the location and

dynamics of spin-labelled probes in soft matter

Quantum effects at muon stopping sites

**15:25 - 15:45:** Matjaž Gomilšek

(Jožef Stefan Institute)

**15:45:** Closing Remarks

(Steve Cottrell)

15:45 – 16:30 Extended break-out rooms