A new, hand-held, 1- to 5-m standoff analyzer for real-time detection of trace chemical, biological, and explosive substances on surfaces

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Agenda

- Description of the Standoff Handheld CBE (SHCBE) Analyzer
- Benefits & opportunities of deep UV Raman & fluorescence detection
- Some results
- Extensions of SHCBE technology

What is the SHCBE 200

SHCBE 200 is a fully self-contained hand-held real-time point-and-shoot analyzer with:

- autofocus telescope for surface targets from 0.6 to 5+ m in full daylight conditions;
- single handed control;
- wide and narrow field of view context images;
- a deep UV laser and control electronics;
- auto-calibrating deep UV Raman & fluorescence spectrometer & other built-in-tests;
- embedded computer with on-board data processing and CBE library; and
- display showing context information and target identification.
- remote Android compatible

The Photon Systems SHCBE 200 analyzer employs two complementary optical methods without any optical interference from ambient light or due to Raman and fluorescence spectral overlap.

Features of SHCBE 200

- **Single handed operation:** 4-button plus trigger control
- **Warm-up:** < 10s from cold start, 3 s from standby mode
- **Built-in-test:** full functional test of all components on startup
- **Spectral Calibration:** Auto-calibrated on analyzer startup
- **Two Coaxial Context Cameras:**
  1) 75^{o} wide angle image;
  2) 20mm micro image centered around laser spot
- **Autofocused Standoff:** based on micro context image
- **Standoff Distance:** 0.5 m to 5+ m in full daylight conditions
- **Spectral Range:** **Raman:** 250 cm^{-1} to 4000cm^{-1}
  Fluorescence: 270nm to 320nm
- **Materials Detected:** Chemical, Biological and Explosives
- **CBE Libraries:** Built in unclassified library +SD card libraries

Other SHCBE 200 Information

- **Context Info with Spectral Data:** Date/time stamps, GPS, azimuth, distance and two images
- **Power Supply:** Replaceable 24 V LiPO battery pack (UN/DOT 38.3 rated) or 24 V wall adapter
- **Communication:** WiFi/Bluetooth (to Android/ATAK), plus Wire
- **Weight:** 12 pounds
- **Dimensions:** 7” W x 11” H x 16” L
- **Battery Lifetime:** >20 hrs in standby, > 200 spectral analyses
- **Display:** Color 1920x1080, 5.9” LCD
- **Ambient:**-40 ^{o}C to +60 ^{o}C, 0-90% humidity, -1 km to +20 km
- **Shock/Vib:** TBD
- **Ingress Protection:** IP65
- **Robot compatible:** ¼ -20 camera thread or dove-tail mount
- **Maintenance:** > 1 year with window clear of debris

Preliminary SHCBE Home &/or ATAK Screen

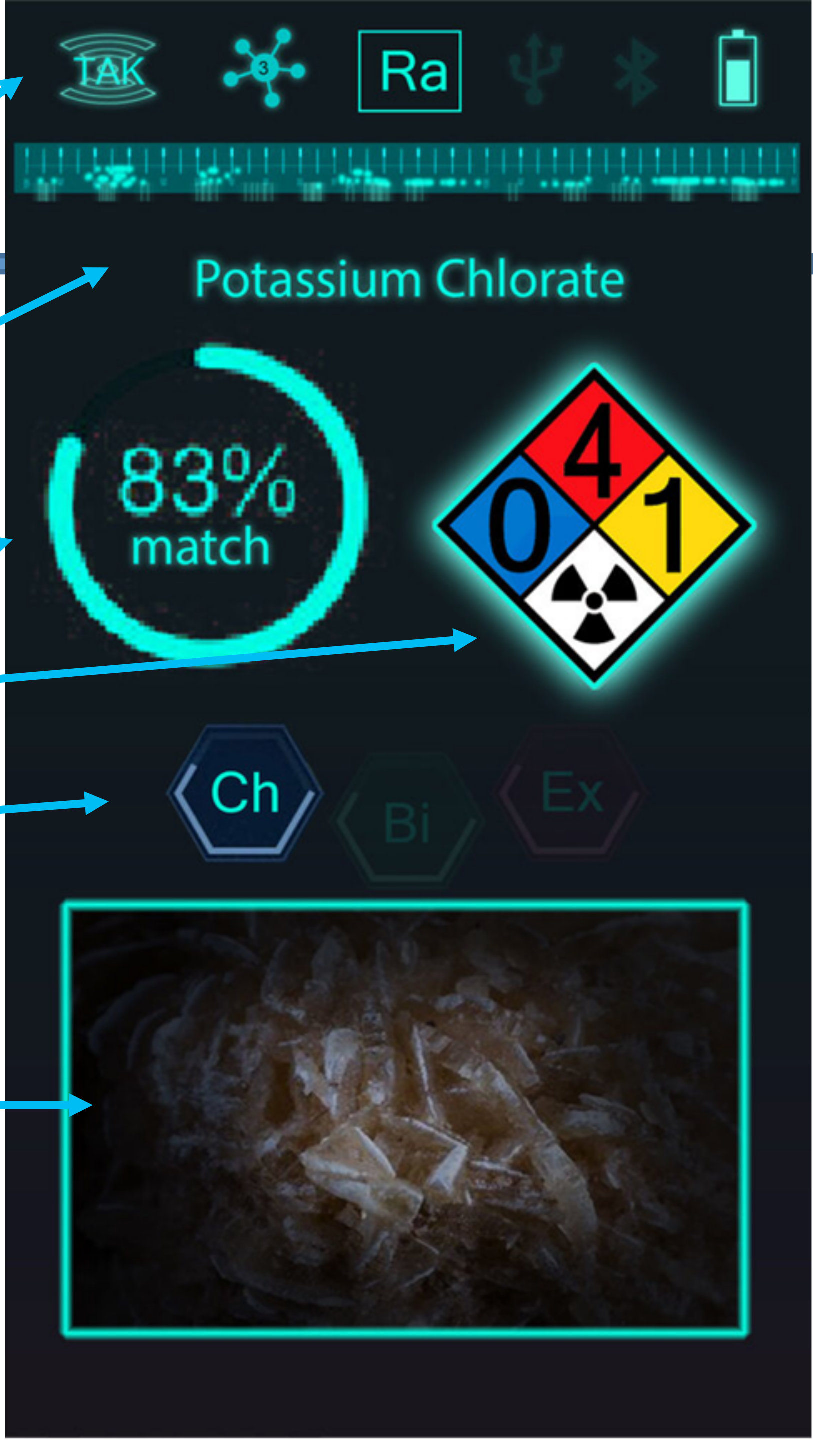
Situational Info w battery status:
Close match time history:

Specific CBE Identification:

Probability of Identification (PID):
& Hazard level:

CBE hazard category:

Micro-context real-time image:



Display Screens
All screens shown on SHCBE &/or ATAK

- **Home Screen**: Default screen for command & control choices & context image
  a) Situational info including: ATAK connection status, date, time, location, battery charge status, distance to target, ready light,
  b) Micro real-time images of targeted area for detection. Macro image captured with data set, but not displayed.
  c) CBE hazard information: Top most probably ID. Possible top three IDs
- **SHCBE Training Screen:**
  a) A baseline set of on-board CBE fluorescence & Raman library materials will be installed in SHCBE
  b) Additional CBE materials will need to be installed in the on-board library. Many or most of these materials are unavailable to PSI for security and hazard reasons. Training screen enables users to conveniently add new CBE materials to the on-board chemical library to enable memory of unusual substance to see if they come up again in other locations.
- **In Depth Screen:**
  a) Perhaps another screen or two to show more details of fault diagnostics and the chemometrics and Euclidian distance relationships in 6D PCA space.
  b) A screen showing the spectral calibration results
  c) A screen showing the target autofocus results.

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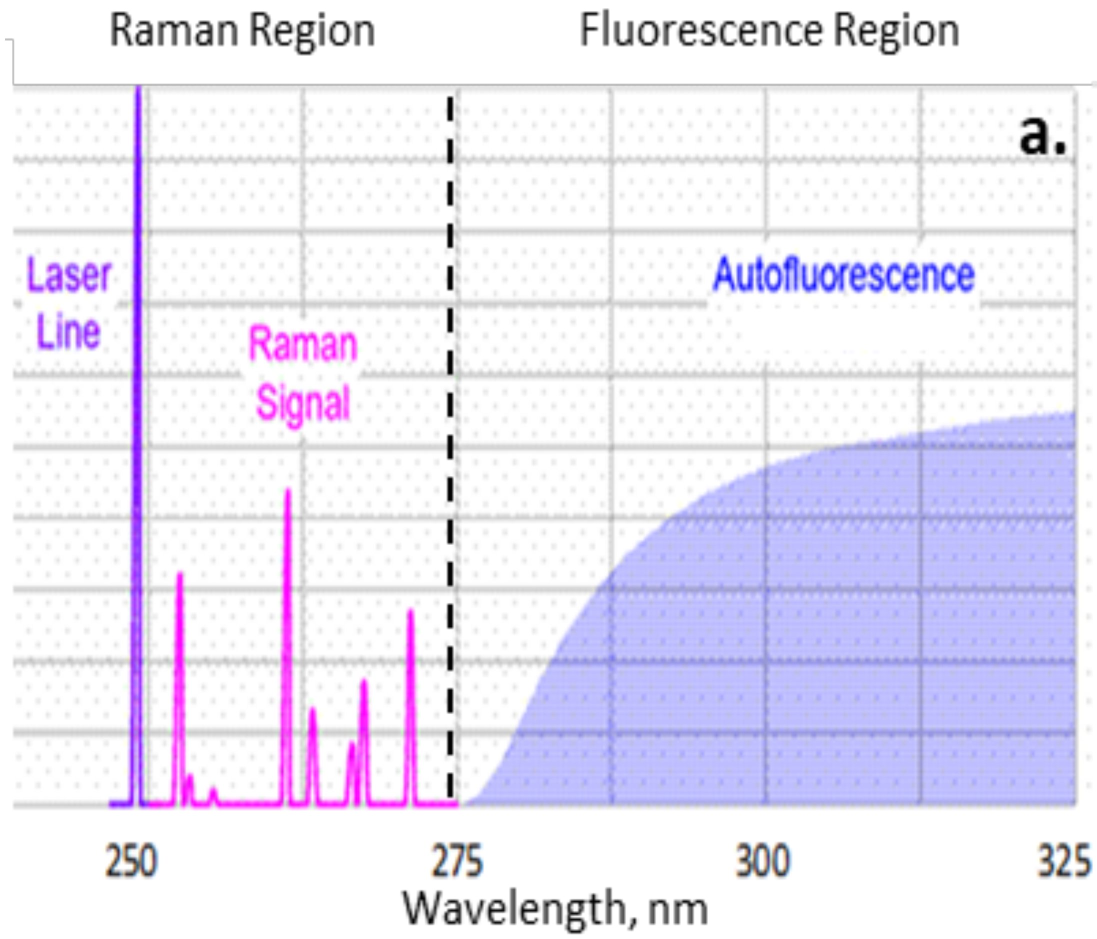
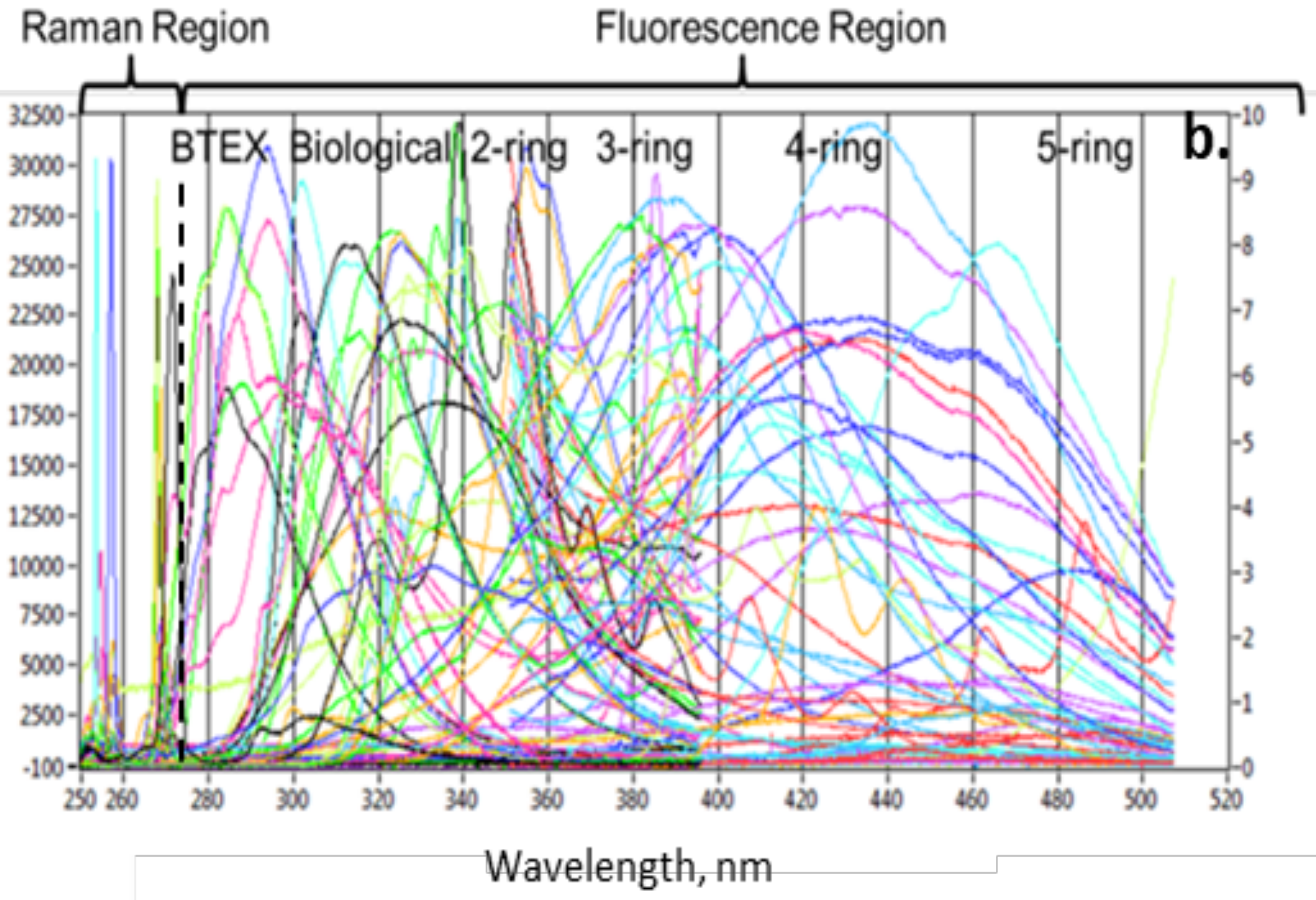
Benefits & Opportunities of Deep UV Methods

- **Solar & artificial light blind, enabling standoff detection:** When excitation occurs below 250 nm, Raman emissions occur within a **solar blind and fluorescence free** region of the spectrum. Raman & fluorescence emissions occur in separate spectral regions.
- **Deep UV excitation enables much higher sensitivity & specificity compared to Raman at visible or IR wavelengths**, as well as enabling detection of the full spectral range of fluorescence emissions from unknown materials, providing enhanced probability of detection and lower false alarm rates.
- **Deep UV excitation has short penetration into samples & enables physical separation of targeted surface material** from substrate or matrix material. Soft DUV pulse method avoids sample damage.
- **Eye & skin hazards are reduced** using deep UV excitation due to lack of penetration of the laser to the retina. Skin hazard nominally no different than sun exposure.
- **Enables the detection of a broad range of biological materials in addition to C & E.**

Separation of Rayleigh, Raman, & Fluorescence
when excitation is < 250 nm

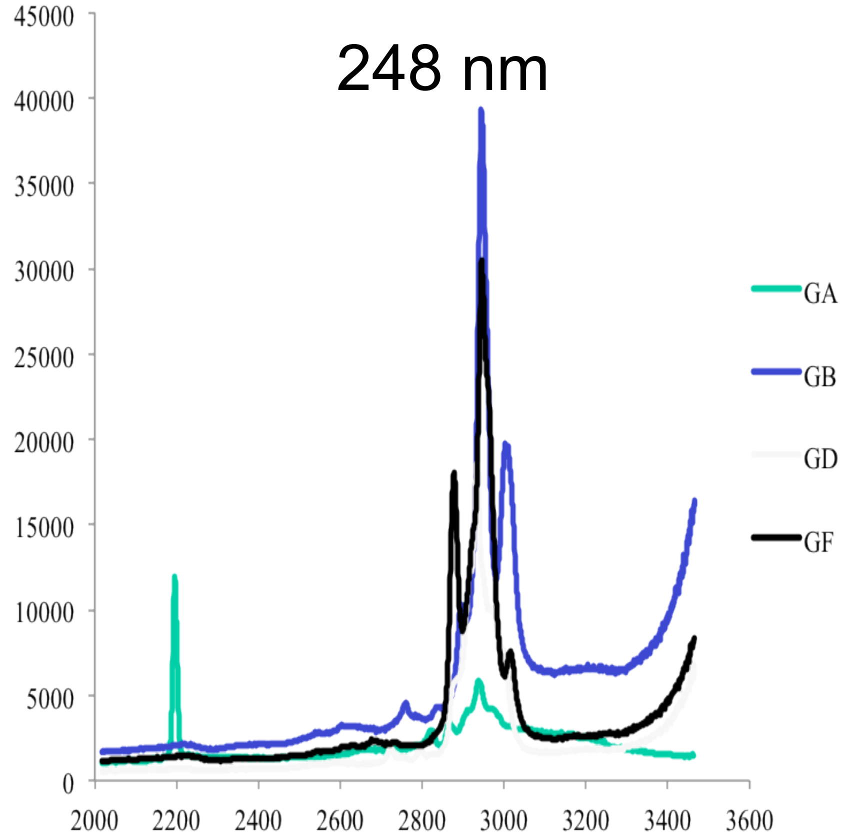


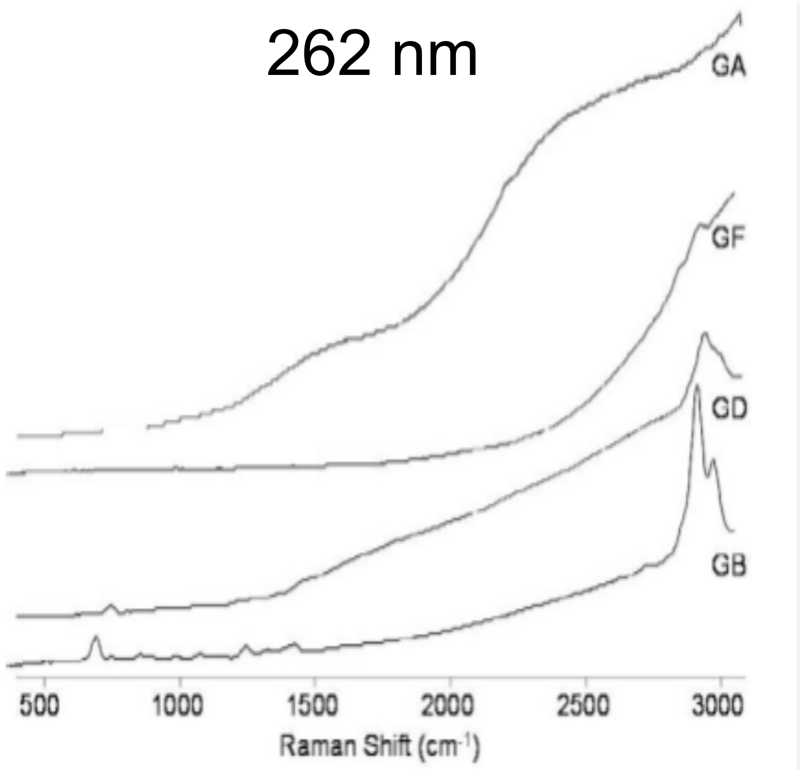


Sensitivity to Excitation Wavelength

Raman Spectra with Excitation at 248 nm versus 262 nm

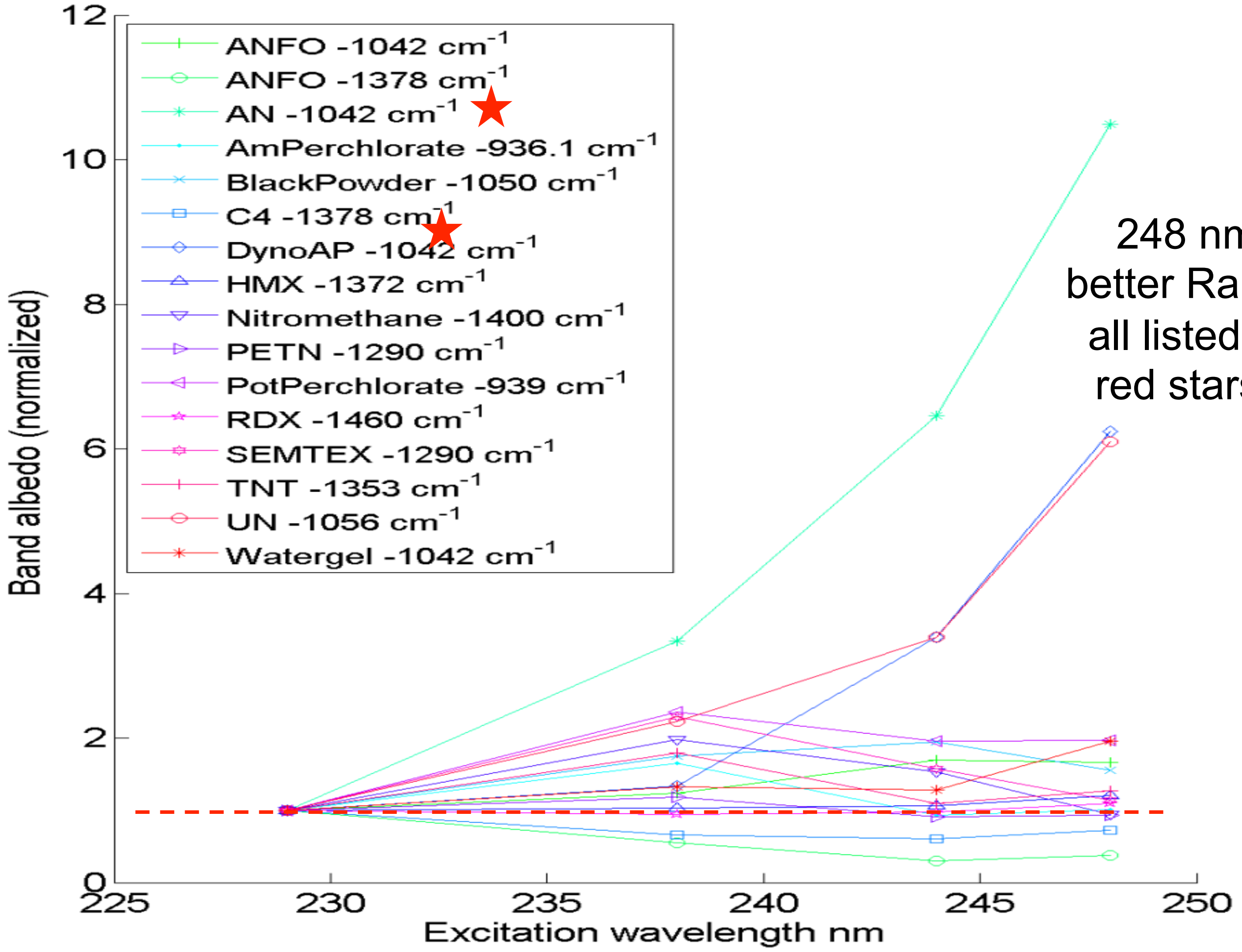
(Example is G Agents)





Adapted from Christesen, SD et al. Appl Spec. 2008 Oct; 62(10):1078-83

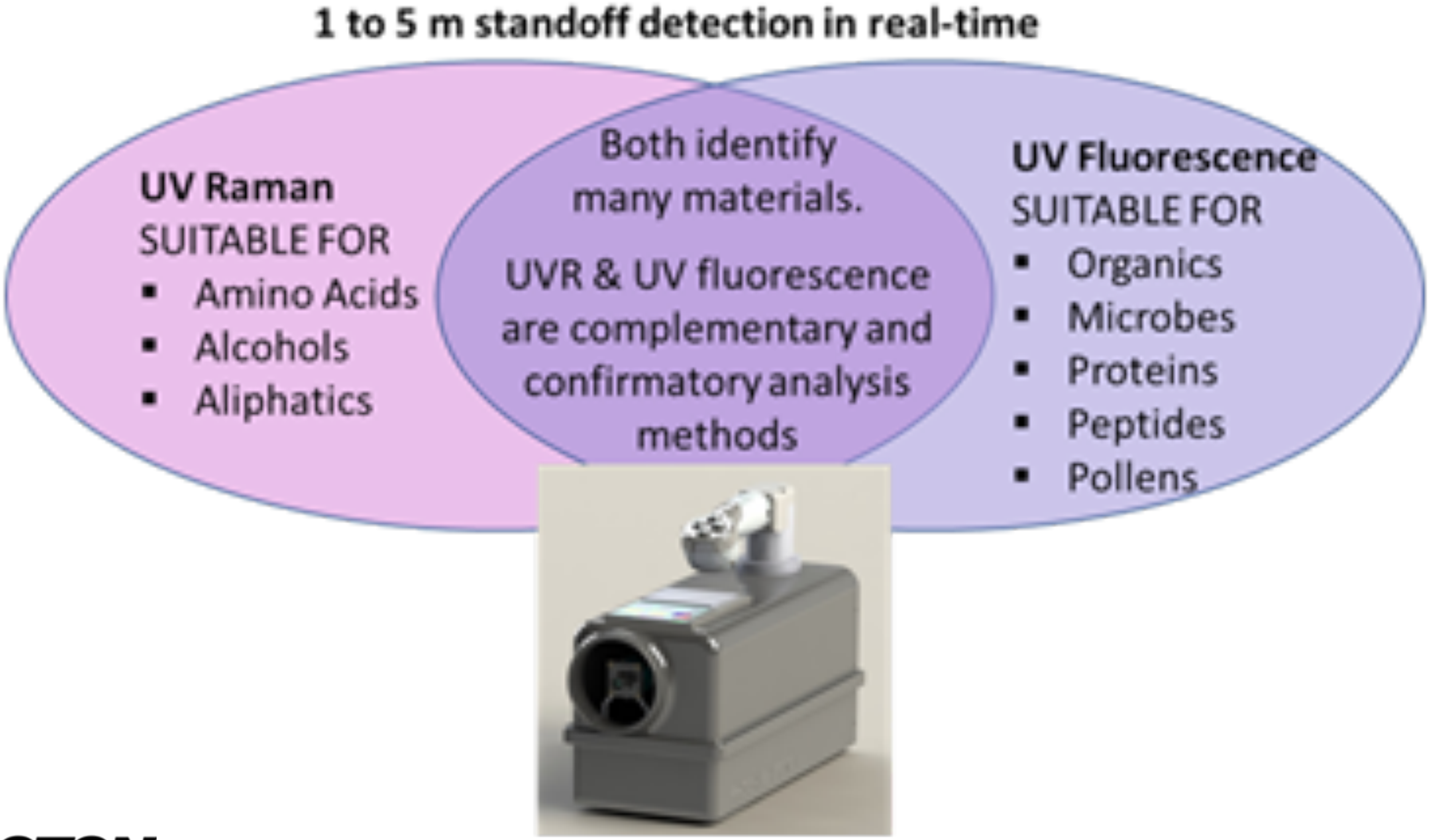
Effect of Wavelength on Raman Albedo



248 nm excitation provides better Raman signal strength for all listed materials except with red stars, i.e. 88% of samples

Yellampalle, et.al., "Multiple-excitation-wavelength resonance Raman explosive detection", SPIE Vol. 8018, West Virginia High Technology Consortium Foundation, May 2011.

Combining the Sensitivity of Fluorescence & Specificity of Raman



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Combining Two Orthogonal Detection Methods: Sensitivity of Fluorescence & Specificity of Raman

- Fluorescence is the most sensitive method of detection, over 10^6 to 10^8 times more sensitive than Raman, providing longer standoff distances and/or detection at lower concentrations

- Fluorescence data provides information about the electronic structure of targeted materials (aromatics, ketones, aldehydes)

- Raman provides information about chemical bonds and functional groups, including those that do not fluoresce (aliphatics and simple compounds)

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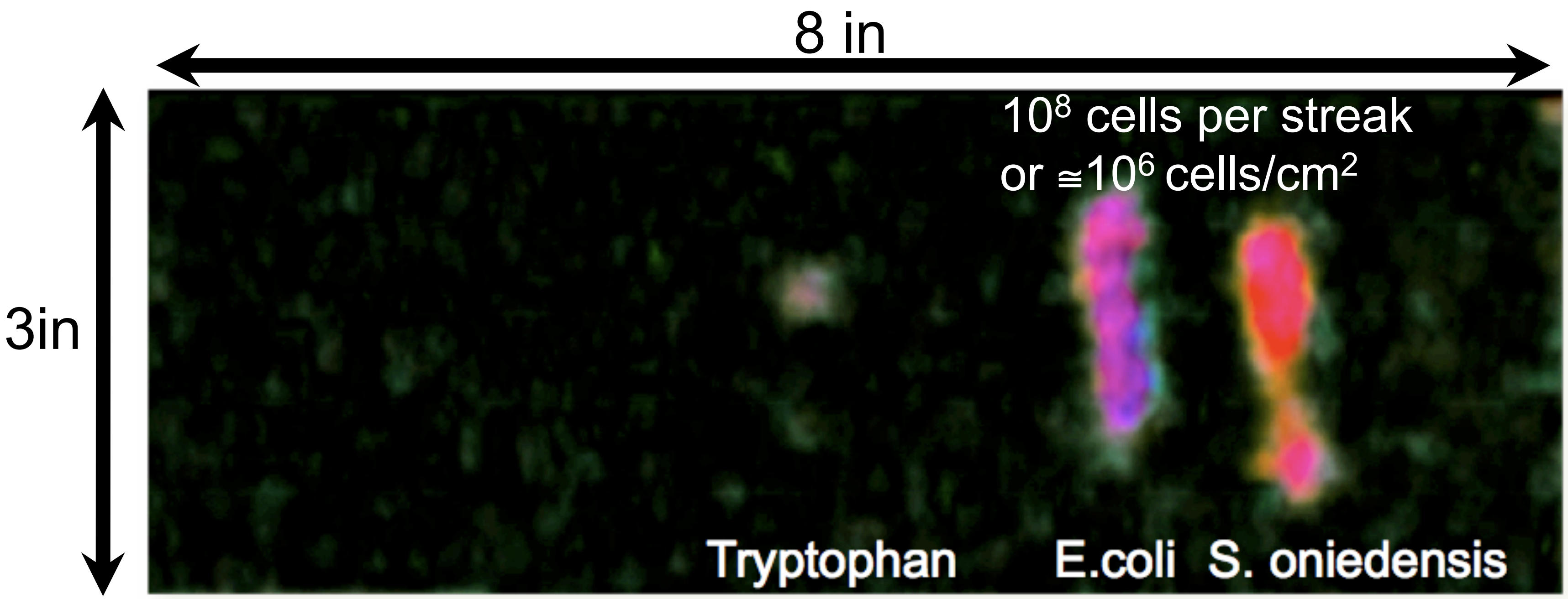
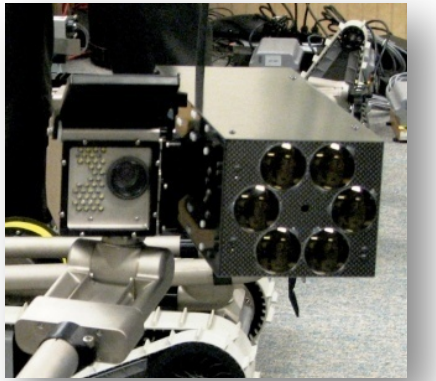
Standoff Microbial Differentiation on Painted Wall

@ 2 m with TUCBE Gen 1.0, @ 6 m with TUCBE Gen 2.0 (f/55)



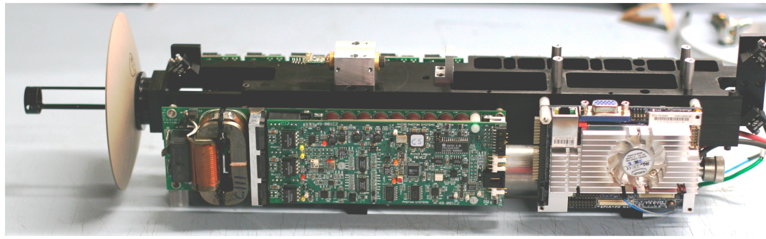
TUCBE Gen 1.0



On PackBot EOD

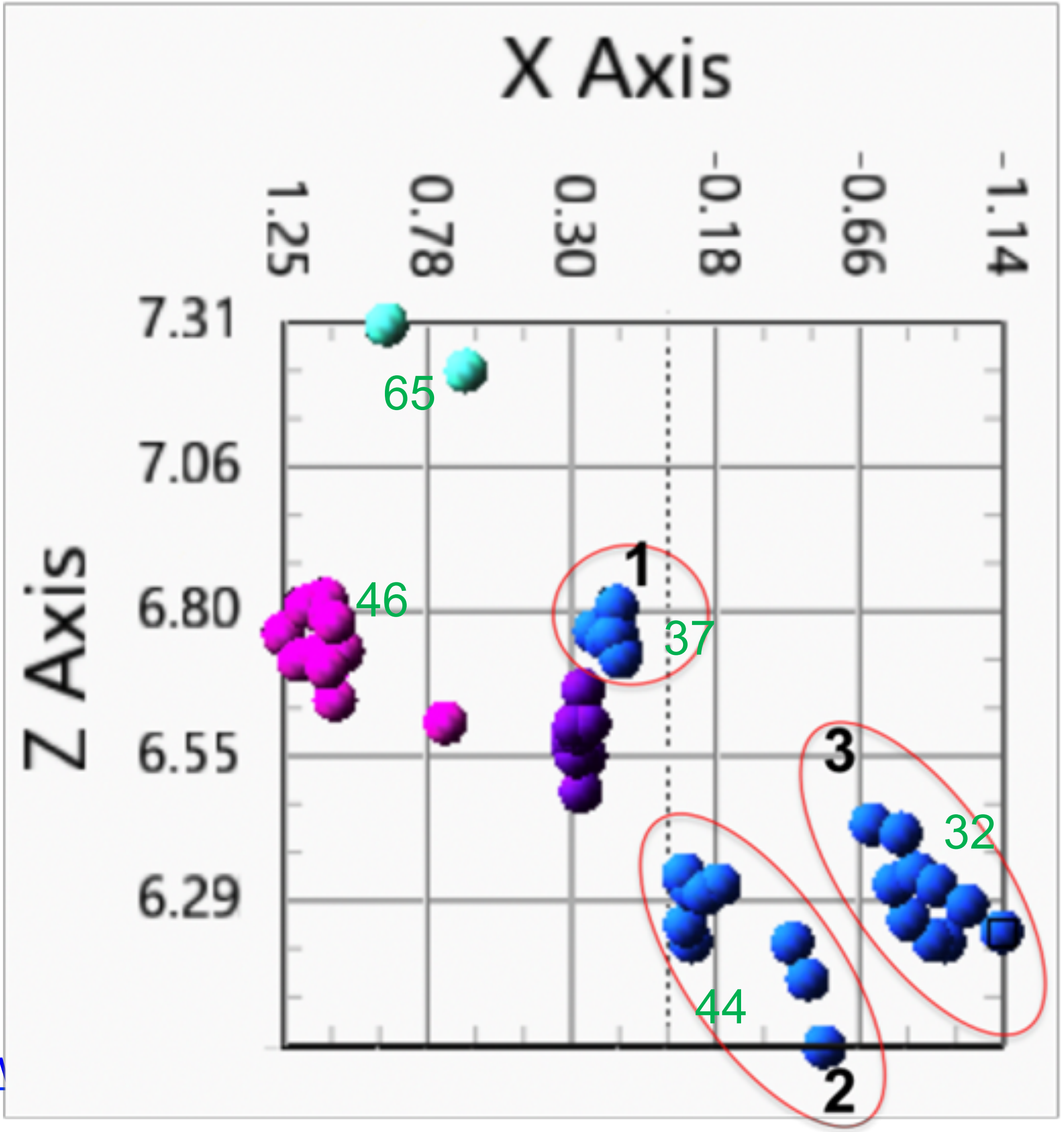
- Differentiability of two gram (-) genuses, due to phenotypic traits associated to protein composition & conformation
- Colors are NOT arbitrary, but determined by conversion of PCA vectors to RGB color intensity

TUCBE Gen 2.0



Genus Level Differentiability of Microbes

- Detection diluted in talc down < 10 microbes in view volume or <1/50K w/w
- Multiple independent preparations and samples per organism



Level 4 Training set: bio samples excluding proteins & yeasts

GC% content shown in green

E. coli
Bacillus sp.
1. B. megaterium
2. B. subtilus
3. B. cereus
S. Oneidensis
P. aruginosa

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Independent CWA/NTA Test

w predecessor DTRA TUCBE Gen 4 Sensor at ECBC (Steve Christesen, Jason Guicheteau, Way Fountain)

Unknown Sample	Matched Material (PSI/JPL Analysis)	Fluorescence Match (%)	Raman Match (%)	ECBC Actuals	Correctly Identified Chem	Correctly Identified Surface
UN01	F_S1	99.44	99.77	F_S1		
UN02	S2	99.93	99.78	S2		
UN03	C_S2	99.95	99.76	C_S2		
UN04	D_S2	99.04	99.67	D_S2		
UN05	E	99.94	99.73	E		
UN06	A	99.86	99.87	A		
UN07	B_S2	95.99	98.76	B_S2		
	UN22	98.35	98.86			
UN08	C_S3	99.94	99.78	C_S3		
UN09	F_S3	92.84	98.43	F_S3		
UN10	H	99.95	99.85	H		
UN11	G	99.96	99.88	G		
UN12	F_S2	96.63	99	F_S2		
UN13	C	99.63	99.8	C		
UN14	D	99.93	99.73	D		
UN15	S1	99.84	99.76	S1		
UN16	B_S1	99.29	99.63	B_S1		
UN17	F	99.97	99.7	F		
UN18	I	99.79	99.73	I		
UN19	S3	99.57	99.62	S3		
UN20	C_S1	99.55	99.76	C_S1		
UN21	D_S3	99.88	99.72	D_S3		
UN22	B_S2	94.35	97.85	B_S3		
	UN07	98.35	98.86			
UN23	B	99.73	99.83	B		
UN24	D_S1	99.62	99.77	D_S1		

24 total samples:
9 different CWAs & NTAs
pure and on
3 different surfaces

100% of the 9 pure samples were correctly identified with a minimum confidence above 99.63%.

Among all 24 blind unknown samples, the match was above 97.85% for Raman matching and above 98.35% for all but 4 unknowns, where the confidence was 96.63%, 95.99%, 94.35%, and 92.84%.

Independent Explosives Test

W predecessor DTRA TUCBE Gen 4 Sensor at IHEODTD (Steve Culfogeinis, et.al.)

	False Positives	False Negatives	Correctly ID'd	N values
Perchlorate	0%	0%	100%	2
Chlorate	0%	0%	100%	2
Ammonium Nitrate	0%	0%	100%	10
Urea Nitrate	0%	0%	100%	1
ANFO	0%	0%	100%	4
Black Powder	0%	0%	100%	6
Smokeless Powder	0%	0%	100%	1
Hydrogen Peroxide	0%	50%	100%	2
Hydroxides	0%	0%	100%	3
C4	0%	0%	100%	7
PE4	0%	0%	100%	4
PETN	0%	0%	100%	11
TNT	0%	0%	100%	11

4 different military grade explosives plus
9 different HME and precursor materials

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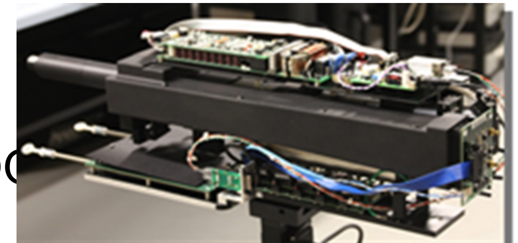

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A Closer Look at the SHCBE 125 Analyzer

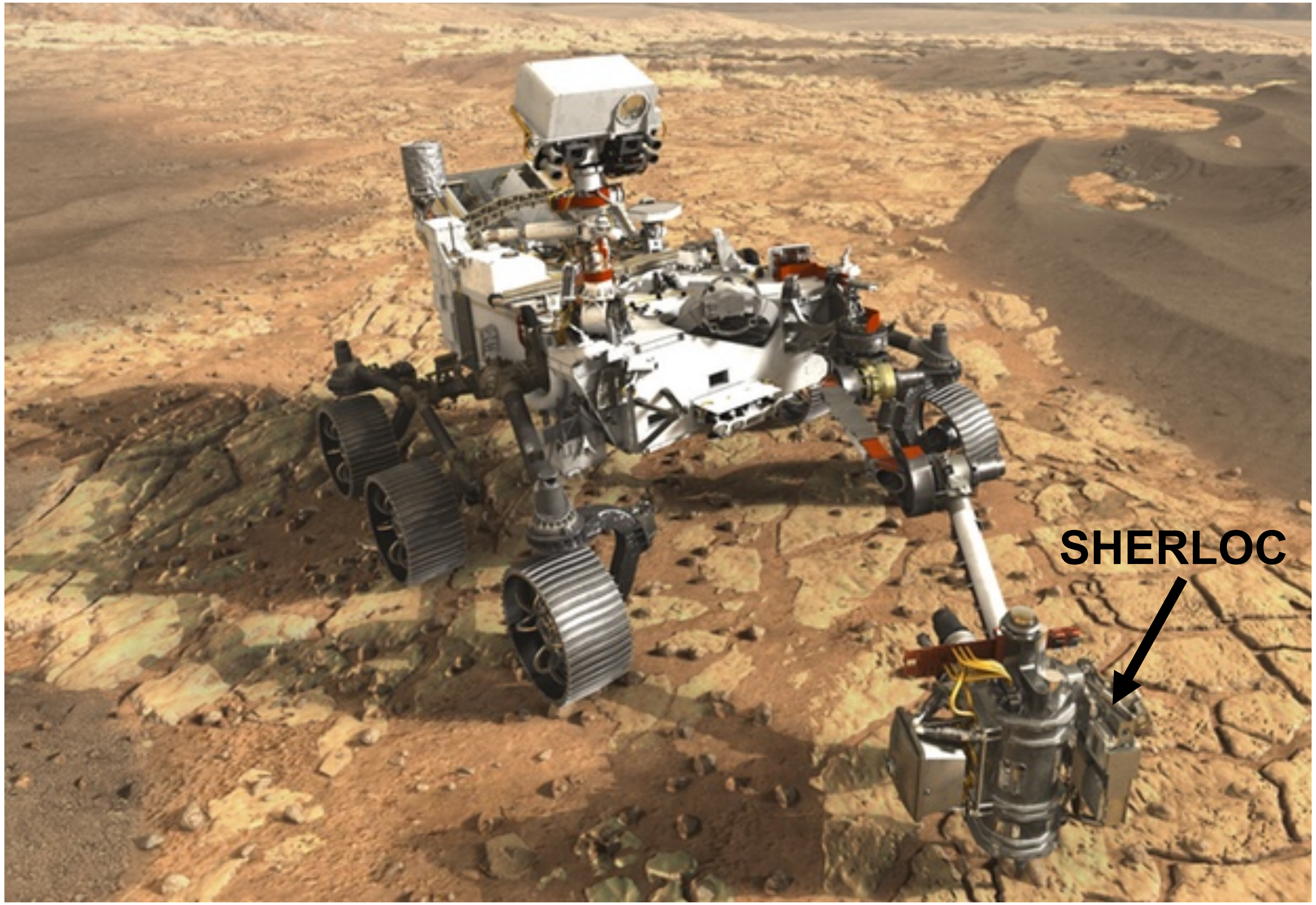
SHCBE 125 Specifications:

✓Detection type: fused deep UV Raman & fluorescence
✓Laser wavelength: 248.6 nm
✓Auto-Focus working distance: 4 cm
✓Bump test calibration: Raman & fluorescence spectral and amplitude
✓Sampling size: < 0.5 mm dia
✓Detection time: < 100 μs for Raman & fluor
✓Sensor warmup time from cold start: < 10 s
✓Size: 4”x7”x14”
✓Weight: < 5 lbs, including battery
✓Battery life: > 16 hours typical
✓Environmental: IP67
✓Command/control/display: large membrane switch control + OLED
✓Alternate command/control/display: via Android phone, ATAK, etc.
✓Context camera with image captures with data sets
✓On-board CBE library

The Mars 2020 Rover

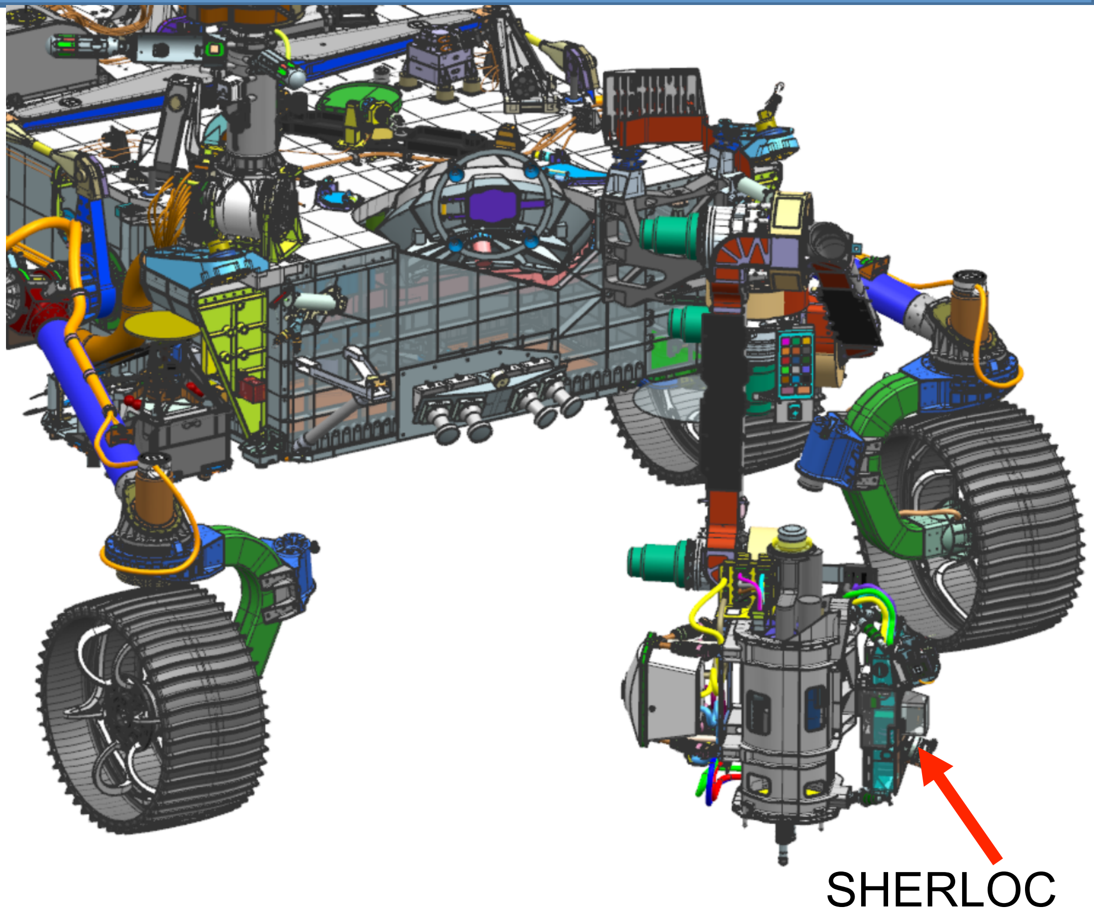
With SHERLOC - a deep UV Raman & fluorescence mapping instrument

Photon Systems and JPL have been working together for over 20 years to develop deep UV Raman and fluorescence spectroscopic methods for detection of organic, prebiotic, and biological materials on Mars and beyond.



The Rover-Arm Mounted Mars 2020 SHERLOC Instrument

- Designed to survive -135C to +70C ambient temperature + take off, cruise, landing, and Mars operations shock/vib.
- SHERLOC produces deep UV Raman & fluorescence chemical images of Martian surfaces, including bore-holes, to detect trace amounts of organic, prebiotic, and biological materials embedded in mineral matrices.
- Mars 2020 is scheduled to launch in August 2020 for landing on Mars 2021.



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